



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:00 PM UTC

PDB ID : 5E5N / pdb_00005e5n
Title : Ketosynthase from module 6 of the bacillaene synthase from *Bacillus subtilis* 168 (C167S mutant, crystal form 1)
Authors : Wagner, D.T.; Gay, D.C.; Keatinge-Clay, A.T.
Deposited on : 2015-10-08
Resolution : 2.00 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

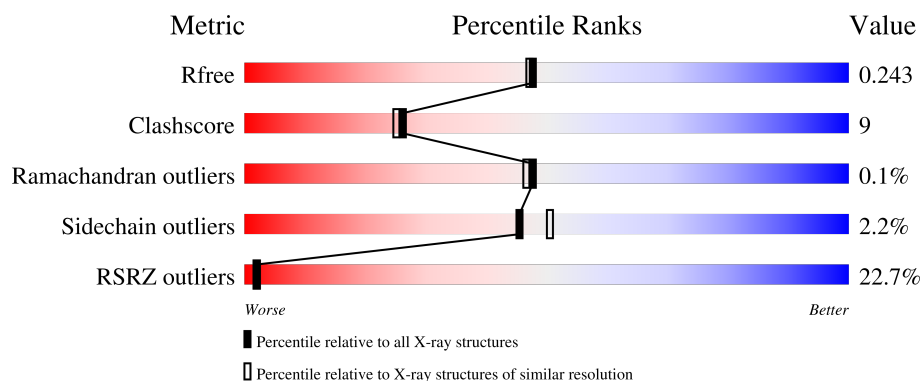
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	617	19% 76% 14% • 9%
1	B	617	19% 76% 15% • 8%
1	C	617	22% 73% 13% • 14%
1	D	617	22% 71% 14% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18597 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 Polyketide synthase PksL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4419	2811	738	845	25			
1	B	568	Total	C	N	O	S	0	0	0
			4461	2837	746	852	26			
1	C	533	Total	C	N	O	S	0	0	0
			4185	2663	703	798	21			
1	D	532	Total	C	N	O	S	0	0	0
			4174	2657	700	796	21			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q05470
A	-20	GLY	-	expression tag	UNP Q05470
A	-19	SER	-	expression tag	UNP Q05470
A	-18	SER	-	expression tag	UNP Q05470
A	-17	HIS	-	expression tag	UNP Q05470
A	-16	HIS	-	expression tag	UNP Q05470
A	-15	HIS	-	expression tag	UNP Q05470
A	-14	HIS	-	expression tag	UNP Q05470
A	-13	HIS	-	expression tag	UNP Q05470
A	-12	HIS	-	expression tag	UNP Q05470
A	-11	SER	-	expression tag	UNP Q05470
A	-10	SER	-	expression tag	UNP Q05470
A	-9	GLY	-	expression tag	UNP Q05470
A	-8	LEU	-	expression tag	UNP Q05470
A	-7	VAL	-	expression tag	UNP Q05470
A	-6	PRO	-	expression tag	UNP Q05470
A	-5	ARG	-	expression tag	UNP Q05470
A	-4	GLY	-	expression tag	UNP Q05470
A	-3	SER	-	expression tag	UNP Q05470
A	-2	SER	-	expression tag	UNP Q05470
A	169	SER	CYS	engineered mutation	UNP Q05470

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	initiating methionine	UNP Q05470
B	-20	GLY	-	expression tag	UNP Q05470
B	-19	SER	-	expression tag	UNP Q05470
B	-18	SER	-	expression tag	UNP Q05470
B	-17	HIS	-	expression tag	UNP Q05470
B	-16	HIS	-	expression tag	UNP Q05470
B	-15	HIS	-	expression tag	UNP Q05470
B	-14	HIS	-	expression tag	UNP Q05470
B	-13	HIS	-	expression tag	UNP Q05470
B	-12	HIS	-	expression tag	UNP Q05470
B	-11	SER	-	expression tag	UNP Q05470
B	-10	SER	-	expression tag	UNP Q05470
B	-9	GLY	-	expression tag	UNP Q05470
B	-8	LEU	-	expression tag	UNP Q05470
B	-7	VAL	-	expression tag	UNP Q05470
B	-6	PRO	-	expression tag	UNP Q05470
B	-5	ARG	-	expression tag	UNP Q05470
B	-4	GLY	-	expression tag	UNP Q05470
B	-3	SER	-	expression tag	UNP Q05470
B	-2	SER	-	expression tag	UNP Q05470
B	169	SER	CYS	engineered mutation	UNP Q05470
C	-21	MET	-	initiating methionine	UNP Q05470
C	-20	GLY	-	expression tag	UNP Q05470
C	-19	SER	-	expression tag	UNP Q05470
C	-18	SER	-	expression tag	UNP Q05470
C	-17	HIS	-	expression tag	UNP Q05470
C	-16	HIS	-	expression tag	UNP Q05470
C	-15	HIS	-	expression tag	UNP Q05470
C	-14	HIS	-	expression tag	UNP Q05470
C	-13	HIS	-	expression tag	UNP Q05470
C	-12	HIS	-	expression tag	UNP Q05470
C	-11	SER	-	expression tag	UNP Q05470
C	-10	SER	-	expression tag	UNP Q05470
C	-9	GLY	-	expression tag	UNP Q05470
C	-8	LEU	-	expression tag	UNP Q05470
C	-7	VAL	-	expression tag	UNP Q05470
C	-6	PRO	-	expression tag	UNP Q05470
C	-5	ARG	-	expression tag	UNP Q05470
C	-4	GLY	-	expression tag	UNP Q05470
C	-3	SER	-	expression tag	UNP Q05470
C	-2	SER	-	expression tag	UNP Q05470
C	169	SER	CYS	engineered mutation	UNP Q05470

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	MET	-	initiating methionine	UNP Q05470
D	-20	GLY	-	expression tag	UNP Q05470
D	-19	SER	-	expression tag	UNP Q05470
D	-18	SER	-	expression tag	UNP Q05470
D	-17	HIS	-	expression tag	UNP Q05470
D	-16	HIS	-	expression tag	UNP Q05470
D	-15	HIS	-	expression tag	UNP Q05470
D	-14	HIS	-	expression tag	UNP Q05470
D	-13	HIS	-	expression tag	UNP Q05470
D	-12	HIS	-	expression tag	UNP Q05470
D	-11	SER	-	expression tag	UNP Q05470
D	-10	SER	-	expression tag	UNP Q05470
D	-9	GLY	-	expression tag	UNP Q05470
D	-8	LEU	-	expression tag	UNP Q05470
D	-7	VAL	-	expression tag	UNP Q05470
D	-6	PRO	-	expression tag	UNP Q05470
D	-5	ARG	-	expression tag	UNP Q05470
D	-4	GLY	-	expression tag	UNP Q05470
D	-3	SER	-	expression tag	UNP Q05470
D	-2	SER	-	expression tag	UNP Q05470
D	169	SER	CYS	engineered mutation	UNP Q05470

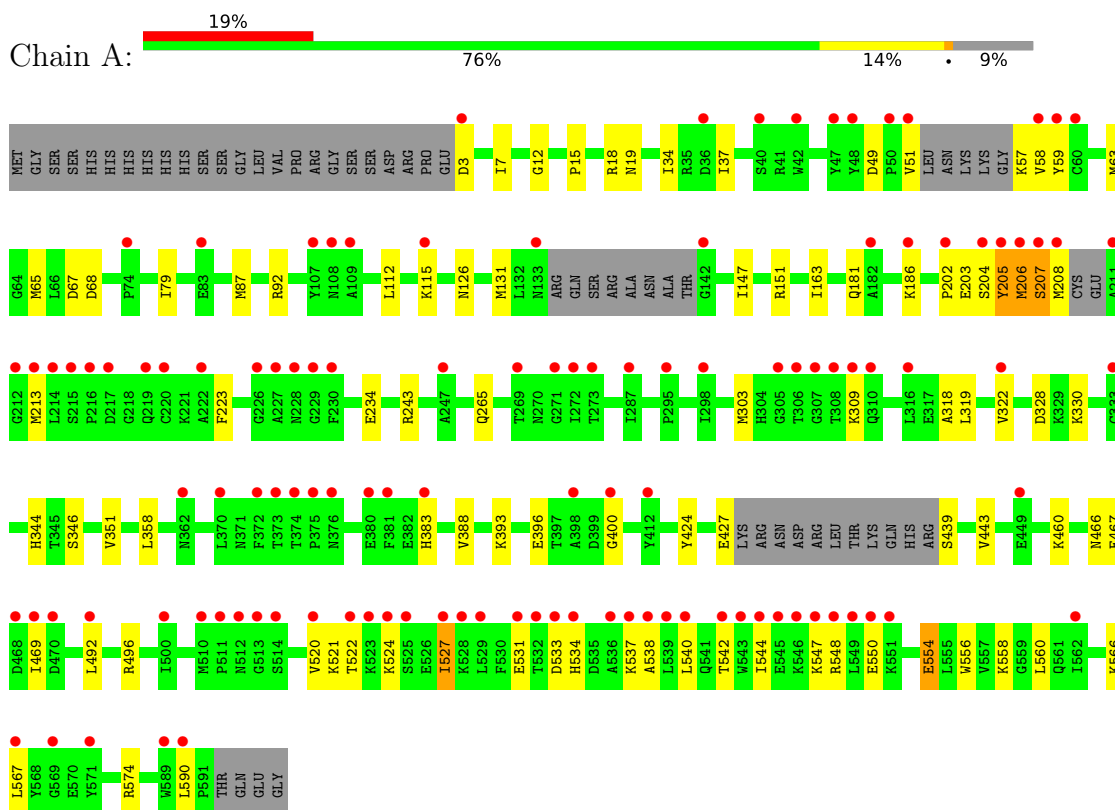
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	371	Total	O	0	0
			371	371		
2	B	333	Total	O	0	0
			333	333		
2	C	320	Total	O	0	0
			320	320		
2	D	334	Total	O	0	0
			334	334		

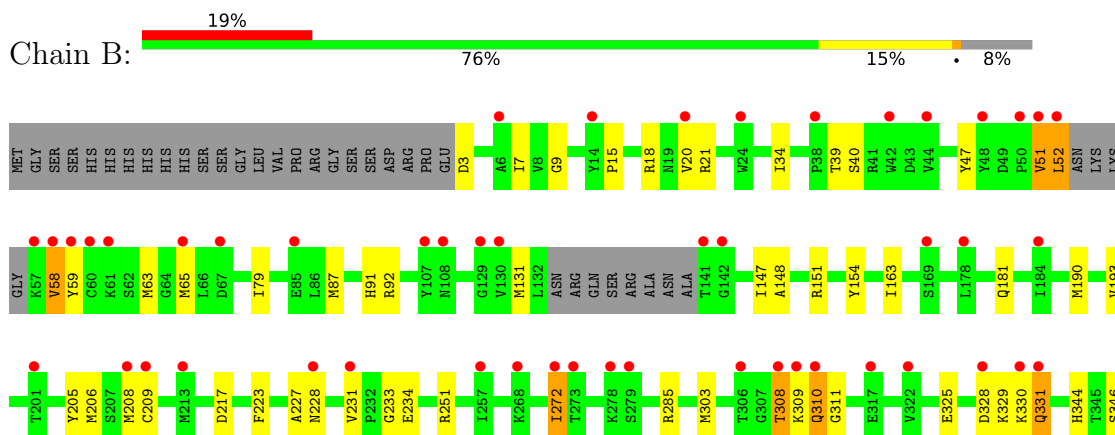
3 Residue-property plots [i](#)

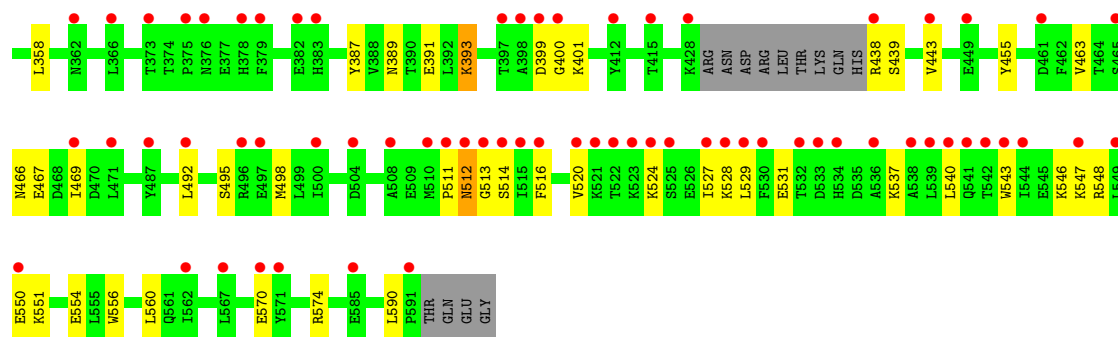
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Polyketide synthase PksL

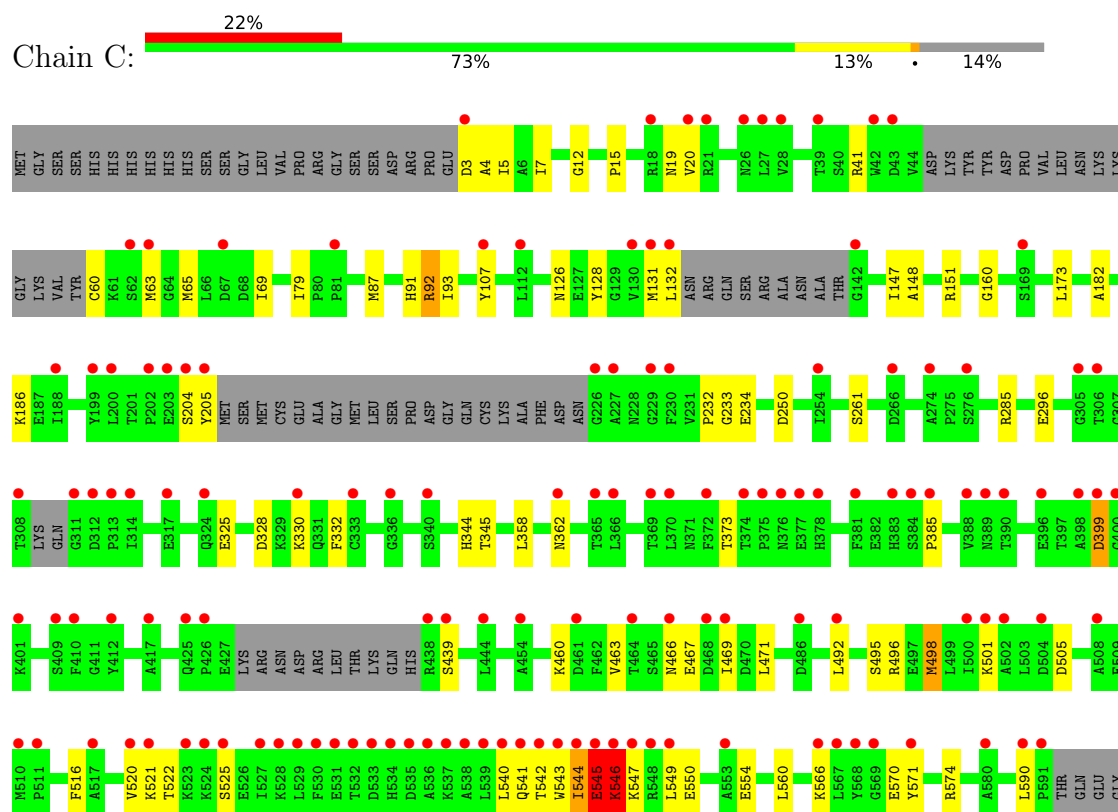


- Molecule 1: Polyketide synthase PksL

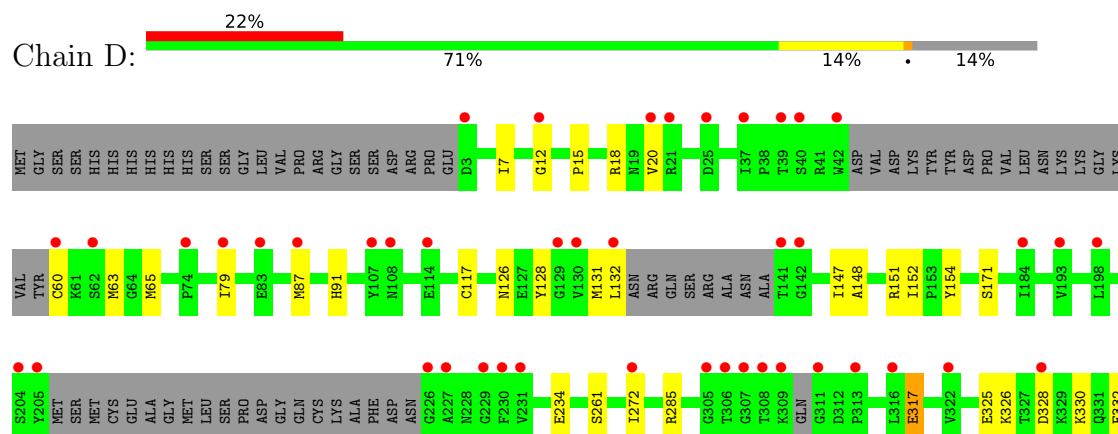


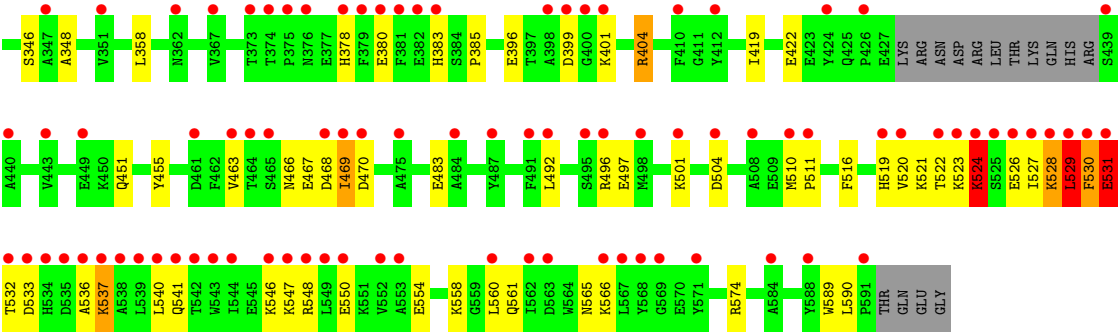


- Molecule 1: Polyketide synthase PksL



- Molecule 1: Polyketide synthase PksL





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.44Å 108.19Å 151.85Å 90.00° 96.43° 90.00°	Depositor
Resolution (Å)	150.00 – 2.00 150.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (150.00-2.00) 99.4 (150.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.202 , 0.236 0.210 , 0.243	Depositor DCC
R_{free} test set	9722 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18597	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.30	9/4518 (0.2%)	0.88	2/6110 (0.0%)
1	B	1.26	10/4561 (0.2%)	0.98	10/6168 (0.2%)
1	C	1.23	9/4277 (0.2%)	0.88	7/5784 (0.1%)
1	D	1.32	12/4266 (0.3%)	0.93	12/5768 (0.2%)
All	All	1.28	40/17622 (0.2%)	0.92	31/23830 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	2
All	All	0	9

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	531	GLU	C-O	8.55	1.33	1.23
1	A	34	ILE	CA-C	7.19	1.60	1.52
1	D	524	LYS	C-O	7.04	1.32	1.24
1	D	404	ARG	CD-NE	-6.72	1.36	1.46
1	D	419	ILE	N-CA	-6.38	1.39	1.46
1	D	529	LEU	C-O	6.36	1.32	1.24
1	B	190	MET	CA-C	6.35	1.60	1.52
1	A	351	VAL	CA-C	6.15	1.60	1.52
1	B	163	ILE	N-CA	-6.10	1.41	1.45
1	D	152	ILE	CA-C	6.03	1.58	1.52
1	A	112	LEU	N-CA	5.93	1.53	1.46
1	C	92	ARG	C-O	-5.90	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	117	CYS	CA-C	-5.87	1.45	1.52
1	D	531	GLU	N-CA	-5.87	1.38	1.46
1	B	9	GLY	C-O	-5.87	1.18	1.24
1	C	93	ILE	C-O	-5.71	1.17	1.24
1	D	171	SER	N-CA	5.66	1.53	1.46
1	B	39	THR	CA-CB	5.61	1.62	1.53
1	A	163	ILE	N-CA	-5.59	1.39	1.46
1	B	193	VAL	C-O	-5.48	1.18	1.24
1	B	231	VAL	CA-C	5.42	1.57	1.52
1	C	182	ALA	CA-C	5.42	1.59	1.52
1	A	206	MET	C-O	-5.39	1.18	1.24
1	B	34	ILE	CA-C	5.31	1.58	1.52
1	B	498	MET	CA-C	5.30	1.59	1.52
1	B	233	GLY	N-CA	-5.29	1.39	1.44
1	C	107	TYR	N-CA	5.27	1.52	1.45
1	A	37	ILE	CA-C	5.24	1.58	1.52
1	D	261	SER	CA-C	-5.18	1.46	1.52
1	A	388	VAL	C-O	-5.18	1.18	1.24
1	A	206	MET	CA-C	-5.17	1.46	1.52
1	C	4	ALA	CA-C	5.17	1.59	1.52
1	B	495	SER	CA-C	-5.16	1.46	1.52
1	D	12	GLY	C-O	5.14	1.29	1.24
1	A	318	ALA	C-O	5.12	1.29	1.24
1	C	5	ILE	C-O	-5.05	1.18	1.24
1	C	498	MET	CA-C	5.05	1.59	1.52
1	D	328	ASP	C-O	-5.03	1.17	1.24
1	C	261	SER	CA-C	-5.01	1.46	1.52
1	C	362	ASN	CA-C	5.01	1.59	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	VAL	CB-CA-C	-23.19	76.28	110.83
1	B	52	LEU	N-CA-CB	-15.21	84.65	110.50
1	B	514	SER	N-CA-CB	-14.71	88.39	110.61
1	D	529	LEU	N-CA-C	13.95	129.40	112.38
1	C	547	LYS	N-CA-C	11.48	127.24	113.23
1	D	531	GLU	N-CA-C	-10.85	96.66	111.96
1	D	531	GLU	CB-CA-C	9.81	128.24	110.88
1	D	529	LEU	CB-CA-C	-9.67	89.92	110.32
1	C	545	GLU	CB-CA-C	-9.41	91.69	110.42
1	C	545	GLU	N-CA-C	9.32	130.66	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	511	PRO	CB-CA-C	-9.19	96.39	111.56
1	B	512	ASN	N-CA-C	9.05	120.56	108.07
1	B	513	GLY	N-CA-C	8.67	133.73	113.18
1	B	512	ASN	N-CA-CB	-8.00	96.53	110.86
1	D	404	ARG	NE-CZ-NH2	7.95	126.36	119.20
1	D	404	ARG	CB-CG-CD	7.93	129.53	111.30
1	C	546	LYS	CB-CA-C	-7.73	99.34	111.17
1	C	399	ASP	CB-CA-C	-7.55	100.21	112.06
1	B	514	SER	N-CA-C	-7.42	103.35	113.30
1	D	530	PHE	N-CA-C	-6.92	105.26	113.21
1	D	469	ILE	CB-CA-C	-6.78	100.32	111.51
1	D	404	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	A	207	SER	N-CA-CB	6.18	120.94	110.49
1	D	126	ASN	CB-CA-C	-5.97	101.86	111.18
1	D	399	ASP	N-CA-C	5.77	119.20	111.24
1	B	399	ASP	N-CA-C	5.71	117.73	108.08
1	A	393	LYS	N-CA-C	5.63	113.29	108.22
1	B	393	LYS	N-CA-C	5.33	114.27	108.14
1	C	549	LEU	N-CA-C	-5.24	105.63	112.23
1	C	126	ASN	CB-CA-C	-5.20	103.06	111.18
1	D	531	GLU	CA-C-O	-5.08	112.91	120.42

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	400	GLY	Peptide
1	A	92	ARG	Sidechain
1	B	227	ALA	Peptide
1	B	400	GLY	Peptide
1	B	92	ARG	Sidechain
1	C	570	GLU	Peptide
1	C	92	ARG	Sidechain
1	D	529	LEU	Mainchain
1	D	531	GLU	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4419	0	4323	87	1
1	B	4461	0	4373	74	0
1	C	4185	0	4102	74	1
1	D	4174	0	4092	95	0
2	A	371	0	0	17	1
2	B	333	0	0	15	1
2	C	320	0	0	21	0
2	D	334	0	0	15	1
All	All	18597	0	16890	320	3

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 9.

All (320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:531:GLU:O	1:D:537:LYS:NZ	1.62	1.29
1:B:467:GLU:CD	2:B:601:HOH:O	1.81	1.23
1:C:542:THR:O	2:C:601:HOH:O	1.55	1.19
1:D:528:LYS:O	1:D:531:GLU:HB3	1.51	1.09
1:D:529:LEU:O	1:D:529:LEU:CD1	2.03	1.07
1:B:79:ILE:HD13	1:B:87:MET:HE1	1.47	0.94
1:D:466:ASN:O	1:D:469:ILE:HD12	1.67	0.94
1:D:528:LYS:O	1:D:531:GLU:CB	2.16	0.94
1:A:79:ILE:HD13	1:A:87:MET:HE1	1.49	0.93
1:A:18:ARG:NH2	2:A:602:HOH:O	2.02	0.93
1:D:531:GLU:C	1:D:537:LYS:HZ3	1.75	0.93
1:C:79:ILE:HD13	1:C:87:MET:HE1	1.51	0.92
1:B:466:ASN:O	1:B:469:ILE:HG13	1.68	0.92
1:C:128:TYR:O	1:C:132:LEU:HD13	1.68	0.92
1:D:79:ILE:HD13	1:D:87:MET:HE1	1.49	0.91
1:D:529:LEU:CD1	1:D:533:ASP:HB2	2.01	0.91
1:A:466:ASN:O	1:A:469:ILE:HG13	1.72	0.89
1:A:58:VAL:HA	1:A:208:MET:HE3	1.54	0.89
1:C:466:ASN:O	1:C:469:ILE:HG13	1.74	0.88
1:D:128:TYR:O	1:D:132:LEU:HD13	1.74	0.88
1:D:529:LEU:O	1:D:529:LEU:HD12	1.71	0.88
1:C:205:TYR:CE1	1:C:232:PRO:HG2	2.09	0.87
1:D:60:CYS:N	2:D:603:HOH:O	2.09	0.86
1:A:208:MET:C	1:A:213:MET:H	1.83	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:LEU:CD1	1:D:533:ASP:CB	2.55	0.85
1:D:532:THR:HA	1:D:537:LYS:HZ1	1.41	0.85
1:D:531:GLU:HA	1:D:531:GLU:OE1	1.75	0.84
1:C:542:THR:HG22	2:C:601:HOH:O	1.77	0.84
1:A:547:LYS:HE3	1:A:567:LEU:O	1.78	0.84
1:D:529:LEU:O	1:D:529:LEU:HD13	1.76	0.83
1:A:396:GLU:OE2	2:A:601:HOH:O	1.96	0.83
1:D:531:GLU:C	1:D:537:LYS:NZ	2.34	0.83
1:A:18:ARG:CZ	2:A:602:HOH:O	2.27	0.82
1:C:541:GLN:O	1:C:545:GLU:HG2	1.81	0.81
1:C:542:THR:C	2:C:601:HOH:O	2.09	0.80
1:D:533:ASP:O	1:D:537:LYS:HG3	1.82	0.80
1:B:52:LEU:CD2	1:B:59:TYR:CD2	2.66	0.79
1:B:52:LEU:HD23	1:B:59:TYR:CD2	2.18	0.78
1:C:501:LYS:HE2	1:C:505:ASP:OD2	1.83	0.78
1:D:483:GLU:OE1	2:D:601:HOH:O	2.01	0.78
1:A:547:LYS:CE	1:A:567:LEU:O	2.31	0.77
1:D:550:GLU:O	1:D:554:GLU:HG3	1.83	0.77
1:C:550:GLU:O	1:C:554:GLU:HG3	1.85	0.76
1:A:550:GLU:O	1:A:554:GLU:HG3	1.84	0.76
1:B:550:GLU:O	1:B:554:GLU:HG3	1.86	0.76
1:A:206:MET:O	1:A:208:MET:HE2	1.86	0.76
1:D:529:LEU:HD11	1:D:533:ASP:HB2	1.67	0.75
1:A:548:ARG:NH2	2:A:603:HOH:O	2.04	0.75
1:A:59:TYR:CE2	1:A:208:MET:HB3	2.21	0.74
1:A:521:LYS:HZ1	1:A:524:LYS:NZ	1.85	0.74
1:A:18:ARG:NE	2:A:602:HOH:O	2.19	0.74
1:A:521:LYS:NZ	1:A:524:LYS:NZ	2.36	0.74
1:C:498:MET:HE1	2:C:625:HOH:O	1.87	0.74
1:D:404:ARG:HD3	1:D:422:GLU:OE2	1.88	0.73
1:C:205:TYR:HE1	1:C:232:PRO:HG2	1.52	0.73
1:C:204:SER:OG	2:C:602:HOH:O	2.06	0.73
1:C:466:ASN:HB2	1:C:469:ILE:HD11	1.71	0.73
1:B:516:PHE:CE1	1:B:554:GLU:HG2	2.24	0.72
1:D:128:TYR:CE2	1:D:132:LEU:HD11	2.25	0.72
1:B:310:GLN:HG3	2:B:703:HOH:O	1.88	0.72
1:D:497:GLU:HG2	1:D:501:LYS:HE2	1.72	0.72
1:A:18:ARG:NH1	2:A:608:HOH:O	2.18	0.72
1:D:565:ASN:OD1	2:D:602:HOH:O	2.08	0.71
1:D:529:LEU:HD13	1:D:533:ASP:HB2	1.71	0.71
1:B:466:ASN:HB2	1:B:469:ILE:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:TRP:C	1:C:545:GLU:H	1.98	0.70
1:A:466:ASN:HB2	1:A:469:ILE:HD11	1.73	0.70
1:A:202:PRO:O	1:A:206:MET:HB2	1.92	0.69
1:A:126:ASN:OD1	2:A:604:HOH:O	2.10	0.69
1:D:531:GLU:O	1:D:537:LYS:CE	2.40	0.69
1:B:272:ILE:HD12	1:D:154:TYR:HB2	1.74	0.69
1:C:205:TYR:CD1	1:C:232:PRO:HG2	2.28	0.69
1:C:128:TYR:CE2	1:C:132:LEU:HD11	2.28	0.68
1:A:427:GLU:O	2:A:605:HOH:O	2.11	0.68
1:D:529:LEU:HD11	1:D:533:ASP:CB	2.22	0.68
1:C:128:TYR:O	1:C:132:LEU:CD1	2.40	0.67
1:D:468:ASP:OD1	2:D:604:HOH:O	2.10	0.67
1:C:542:THR:HA	1:C:545:GLU:HG3	1.74	0.67
1:A:527:ILE:HD11	1:A:558:LYS:HB2	1.75	0.67
1:A:550:GLU:O	1:A:554:GLU:CG	2.42	0.67
1:A:460:LYS:NZ	2:A:611:HOH:O	2.27	0.66
1:C:571:TYR:OH	2:C:604:HOH:O	2.14	0.66
1:D:566:LYS:O	2:D:605:HOH:O	2.12	0.66
1:C:296:GLU:OE2	2:C:603:HOH:O	2.13	0.66
1:A:58:VAL:CA	1:A:208:MET:HE3	2.25	0.65
1:B:328:ASP:O	1:B:330:LYS:HE3	1.96	0.65
1:D:523:LYS:CD	1:D:558:LYS:HG2	2.26	0.65
1:B:574:ARG:NH2	2:B:603:HOH:O	2.23	0.65
1:A:521:LYS:HZ1	1:A:524:LYS:HZ1	1.42	0.65
1:C:250:ASP:OD2	2:C:605:HOH:O	2.15	0.65
1:D:128:TYR:O	1:D:132:LEU:CD1	2.44	0.65
1:A:67:ASP:OD1	2:A:607:HOH:O	2.15	0.65
1:A:527:ILE:CD1	1:A:558:LYS:HB3	2.26	0.65
1:C:541:GLN:O	1:C:545:GLU:CG	2.44	0.65
1:B:546:LYS:HE3	1:B:548:ARG:NH1	2.12	0.64
1:D:529:LEU:CD1	1:D:533:ASP:HB3	2.26	0.64
1:A:49:ASP:HB2	1:A:57:LYS:HD3	1.79	0.63
1:A:460:LYS:HE2	2:A:611:HOH:O	1.98	0.63
1:B:531:GLU:O	1:B:537:LYS:NZ	2.28	0.63
1:C:498:MET:HE2	2:C:814:HOH:O	1.98	0.63
1:D:523:LYS:HD3	1:D:558:LYS:HG2	1.80	0.63
1:B:21:ARG:CZ	2:B:609:HOH:O	2.47	0.63
1:C:128:TYR:CD2	1:C:132:LEU:HD11	2.34	0.63
1:B:21:ARG:NH1	2:B:609:HOH:O	2.31	0.62
1:D:317:GLU:HB3	2:D:755:HOH:O	1.99	0.62
1:B:217:ASP:OD2	1:B:228:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:LYS:HB2	2:C:601:HOH:O	1.97	0.62
1:D:540:LEU:HD22	1:D:560:LEU:HD21	1.82	0.62
1:B:540:LEU:HD22	1:B:560:LEU:HD21	1.81	0.62
1:D:546:LYS:HE3	1:D:548:ARG:HH21	1.64	0.62
1:A:538:ALA:O	1:A:542:THR:HG23	2.00	0.61
1:B:543:TRP:CE2	1:B:551:LYS:HD2	2.35	0.61
1:B:546:LYS:CD	1:B:546:LYS:O	2.48	0.61
1:A:547:LYS:HE3	1:A:567:LEU:C	2.24	0.61
1:B:47:TYR:CD1	1:B:206:MET:CE	2.84	0.61
1:B:546:LYS:O	1:B:546:LYS:HD2	2.00	0.61
1:A:205:TYR:CD1	1:A:205:TYR:C	2.78	0.60
1:A:540:LEU:HD22	1:A:560:LEU:HD21	1.81	0.60
1:B:467:GLU:CG	2:B:601:HOH:O	2.28	0.60
1:D:326:LYS:NZ	2:D:608:HOH:O	2.28	0.60
1:D:529:LEU:C	1:D:531:GLU:H	2.08	0.60
1:D:128:TYR:CD2	1:D:132:LEU:HD11	2.36	0.60
1:B:147:ILE:HD12	1:D:272:ILE:HD13	1.83	0.60
1:C:516:PHE:CE1	1:C:554:GLU:HG2	2.36	0.60
1:B:546:LYS:O	1:B:546:LYS:CG	2.49	0.59
1:C:498:MET:CE	2:C:814:HOH:O	2.50	0.59
1:C:540:LEU:HD22	1:C:560:LEU:HD21	1.84	0.59
1:A:131:MET:HE2	1:A:590:LEU:HD11	1.85	0.59
1:B:3:ASP:N	2:B:613:HOH:O	2.36	0.59
1:A:208:MET:C	1:A:213:MET:N	2.60	0.58
1:A:527:ILE:CD1	1:A:558:LYS:CB	2.81	0.58
1:A:383:HIS:CE1	2:A:617:HOH:O	2.57	0.57
1:C:131:MET:HE2	1:C:590:LEU:HD11	1.87	0.57
1:A:460:LYS:CE	2:A:611:HOH:O	2.52	0.57
1:C:543:TRP:C	1:C:545:GLU:N	2.57	0.57
1:A:521:LYS:NZ	1:A:524:LYS:HZ3	2.01	0.57
1:D:131:MET:HE2	1:D:590:LEU:HD11	1.86	0.57
1:B:51:VAL:HG12	1:B:52:LEU:N	2.19	0.56
1:B:131:MET:HE2	1:B:590:LEU:HD11	1.86	0.56
1:B:391:GLU:HG3	1:B:393:LYS:HD3	1.88	0.56
1:C:132:LEU:HD12	1:C:590:LEU:HD21	1.88	0.56
1:C:132:LEU:HD12	1:C:590:LEU:CD2	2.36	0.56
1:D:530:PHE:O	1:D:560:LEU:HD11	2.06	0.56
1:A:49:ASP:CB	1:A:57:LYS:HD3	2.36	0.55
1:A:547:LYS:HE2	1:A:567:LEU:O	2.05	0.55
1:A:204:SER:OG	1:A:205:TYR:N	2.38	0.55
1:D:497:GLU:CG	1:D:501:LYS:HE2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:537:LYS:O	1:D:541:GLN:HG3	2.07	0.55
1:D:529:LEU:HD12	1:D:536:ALA:HB2	1.88	0.55
1:D:528:LYS:O	1:D:531:GLU:HB2	2.06	0.55
1:A:527:ILE:HD11	1:A:558:LYS:CB	2.35	0.55
1:D:519:HIS:O	1:D:522:THR:OG1	2.19	0.55
1:B:546:LYS:O	1:B:546:LYS:HG3	2.06	0.54
1:D:466:ASN:O	1:D:469:ILE:CD1	2.48	0.54
1:A:58:VAL:CB	1:A:208:MET:HE3	2.37	0.54
1:C:492:LEU:HD12	1:C:492:LEU:N	2.22	0.54
1:A:186:LYS:HD2	1:A:243:ARG:CZ	2.38	0.54
1:B:272:ILE:CD1	1:D:154:TYR:HB2	2.38	0.54
1:D:132:LEU:HD12	1:D:590:LEU:HD21	1.90	0.53
1:B:272:ILE:HD12	1:D:154:TYR:CB	2.39	0.53
1:D:516:PHE:CE2	1:D:554:GLU:HG2	2.43	0.53
1:C:544:ILE:O	1:C:544:ILE:HG22	2.09	0.53
1:D:380:GLU:H	1:D:380:GLU:CD	2.16	0.53
1:D:523:LYS:HD2	1:D:558:LYS:HG2	1.91	0.53
1:A:527:ILE:HD13	1:A:558:LYS:HB3	1.91	0.52
1:B:18:ARG:NH2	2:B:605:HOH:O	2.26	0.52
1:C:60:CYS:N	2:C:618:HOH:O	2.41	0.52
1:B:344:HIS:HD2	1:B:346:SER:H	1.58	0.52
1:C:543:TRP:O	1:C:545:GLU:N	2.41	0.52
1:D:132:LEU:HD12	1:D:590:LEU:CD2	2.39	0.52
1:B:331:GLN:HG3	1:B:387:TYR:HB3	1.90	0.52
1:C:574:ARG:NH2	2:C:617:HOH:O	2.41	0.52
1:D:378:HIS:HD2	2:D:881:HOH:O	1.92	0.52
1:B:272:ILE:HD12	1:D:154:TYR:CG	2.44	0.51
1:C:205:TYR:HE1	1:C:232:PRO:CG	2.20	0.51
1:D:463:VAL:HA	1:D:469:ILE:HD11	1.92	0.51
1:D:524:LYS:O	1:D:528:LYS:HG2	2.11	0.51
1:A:115:LYS:HG2	2:A:851:HOH:O	2.10	0.51
1:D:380:GLU:OE1	1:D:380:GLU:N	2.41	0.50
1:A:206:MET:O	1:A:208:MET:N	2.44	0.50
1:B:40:SER:OG	1:C:328:ASP:OD1	2.14	0.50
1:B:272:ILE:HG13	1:B:272:ILE:O	2.12	0.50
1:C:498:MET:CE	2:C:625:HOH:O	2.55	0.49
1:C:373:THR:HG23	2:C:791:HOH:O	2.11	0.49
1:A:49:ASP:OD1	1:A:51:VAL:HG22	2.12	0.49
1:D:547:LYS:NZ	2:D:605:HOH:O	2.42	0.49
1:C:542:THR:CA	1:C:545:GLU:HG3	2.39	0.49
1:D:531:GLU:C	1:D:537:LYS:HZ1	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG21	1:B:205:TYR:HB3	1.94	0.49
1:B:58:VAL:HG22	1:B:209:CYS:SG	2.53	0.49
1:B:527:ILE:HD12	1:B:531:GLU:OE2	2.12	0.49
1:D:529:LEU:HD13	1:D:533:ASP:CB	2.33	0.49
1:C:15:PRO:HD3	1:C:234:GLU:O	2.13	0.48
1:A:15:PRO:HD3	1:A:234:GLU:O	2.13	0.48
1:B:15:PRO:HD3	1:B:234:GLU:O	2.13	0.48
1:D:510:MET:HE3	1:D:511:PRO:O	2.13	0.48
1:B:63:MET:SD	1:B:65:MET:HG2	2.53	0.48
1:D:15:PRO:HD3	1:D:234:GLU:O	2.13	0.48
1:D:529:LEU:HD12	1:D:536:ALA:CB	2.44	0.48
1:D:533:ASP:O	1:D:537:LYS:CG	2.58	0.48
1:A:344:HIS:CD2	1:A:346:SER:H	2.32	0.48
1:C:542:THR:O	1:C:545:GLU:HG3	2.13	0.48
1:C:467:GLU:HA	1:C:496:ARG:NE	2.29	0.47
1:D:378:HIS:CD2	2:D:881:HOH:O	2.67	0.47
1:D:467:GLU:HG2	1:D:496:ARG:NH2	2.29	0.47
1:A:424:TYR:O	2:A:609:HOH:O	2.20	0.47
1:A:531:GLU:C	1:A:537:LYS:HE3	2.39	0.47
1:B:329:LYS:HG2	2:B:602:HOH:O	2.14	0.47
1:D:63:MET:SD	1:D:65:MET:HG2	2.55	0.47
1:D:128:TYR:CD2	1:D:132:LEU:CD1	2.96	0.47
1:A:265:GLN:HB2	1:C:160:GLY:O	2.14	0.47
1:D:492:LEU:N	1:D:492:LEU:HD12	2.29	0.47
1:B:147:ILE:CD1	1:D:272:ILE:HD13	2.45	0.47
1:C:173:LEU:HB2	2:C:648:HOH:O	2.14	0.47
1:A:204:SER:C	1:A:206:MET:N	2.73	0.46
1:B:52:LEU:CD2	1:B:59:TYR:CE2	2.98	0.46
1:C:128:TYR:CD2	1:C:132:LEU:CD1	2.97	0.46
1:D:332:PHE:CE2	1:D:385:PRO:HB3	2.50	0.46
1:A:492:LEU:N	1:A:492:LEU:HD12	2.31	0.46
1:B:344:HIS:CD2	1:B:346:SER:H	2.32	0.46
1:A:18:ARG:NH2	1:A:68:ASP:OD2	2.48	0.46
1:C:544:ILE:HG21	1:C:566:LYS:HB2	1.98	0.46
1:D:469:ILE:HG22	1:D:470:ASP:C	2.41	0.46
1:A:204:SER:O	1:A:205:TYR:C	2.59	0.46
1:B:492:LEU:HD12	1:B:492:LEU:N	2.30	0.46
1:C:63:MET:SD	1:C:65:MET:HG2	2.56	0.46
1:B:467:GLU:HG3	2:B:601:HOH:O	2.05	0.45
1:B:570:GLU:CD	1:B:570:GLU:H	2.24	0.45
1:C:471:LEU:HD11	1:C:495:SER:C	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:LYS:HD2	2:C:621:HOH:O	2.17	0.45
1:D:7:ILE:HD13	1:D:358:LEU:HD11	1.98	0.45
1:A:58:VAL:HB	1:A:208:MET:CE	2.47	0.45
1:A:147:ILE:O	1:A:151:ARG:HG2	2.16	0.45
1:C:147:ILE:O	1:C:151:ARG:HG2	2.15	0.45
1:A:467:GLU:HA	1:A:496:ARG:NE	2.31	0.45
1:B:272:ILE:HD12	1:D:154:TYR:CD1	2.50	0.45
1:A:206:MET:O	1:A:207:SER:C	2.53	0.45
1:A:443:VAL:HB	1:A:556:TRP:CZ3	2.52	0.45
1:C:41:ARG:NH2	1:C:69:ILE:HD13	2.32	0.45
1:C:344:HIS:HE1	2:C:853:HOH:O	2.00	0.45
1:D:285:ARG:HD3	1:D:325:GLU:OE1	2.17	0.45
1:D:467:GLU:HA	1:D:496:ARG:NE	2.31	0.44
1:A:531:GLU:O	1:A:537:LYS:CE	2.65	0.44
1:B:251:ARG:HD3	2:B:886:HOH:O	2.17	0.44
1:D:532:THR:CA	1:D:537:LYS:HZ1	2.21	0.44
1:A:206:MET:HA	1:A:208:MET:HE2	1.98	0.44
1:A:223:PHE:CZ	1:A:303:MET:HG3	2.52	0.44
1:A:319:LEU:O	1:A:322:VAL:HG22	2.18	0.44
1:D:451:GLN:NE2	2:D:613:HOH:O	2.32	0.44
1:A:79:ILE:CD1	1:A:87:MET:HE1	2.36	0.44
1:C:79:ILE:CD1	1:C:87:MET:HE1	2.36	0.44
1:B:547:LYS:NZ	2:B:628:HOH:O	2.50	0.44
1:D:574:ARG:NH2	2:D:631:HOH:O	2.49	0.44
1:D:574:ARG:NH1	2:D:634:HOH:O	2.51	0.44
1:B:154:TYR:CG	1:D:272:ILE:HG22	2.52	0.43
1:C:132:LEU:CD1	1:C:590:LEU:CD2	2.97	0.43
1:A:574:ARG:NH2	2:A:621:HOH:O	2.44	0.43
1:B:208:MET:HE3	2:B:917:HOH:O	2.18	0.43
1:B:463:VAL:HA	1:B:469:ILE:CD1	2.49	0.43
1:A:58:VAL:HB	1:A:208:MET:HE1	2.00	0.43
1:B:7:ILE:HD13	1:B:358:LEU:HD11	2.01	0.43
1:B:147:ILE:O	1:B:151:ARG:HG2	2.18	0.43
1:C:501:LYS:HE2	1:C:505:ASP:CG	2.44	0.43
1:C:233:GLY:O	1:C:345:THR:HA	2.19	0.43
1:A:7:ILE:HD13	1:A:358:LEU:HD11	2.00	0.43
1:B:330:LYS:O	2:B:602:HOH:O	2.21	0.43
1:D:147:ILE:O	1:D:151:ARG:HG2	2.17	0.43
1:B:308:THR:HG23	1:B:311:GLY:H	1.83	0.43
1:A:344:HIS:HD2	1:A:346:SER:H	1.66	0.43
1:B:389:ASN:OD1	1:B:391:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ARG:HD3	1:B:325:GLU:OE1	2.19	0.43
1:D:532:THR:HA	1:D:537:LYS:NZ	2.23	0.43
1:C:3:ASP:HA	2:C:664:HOH:O	2.17	0.42
1:A:548:ARG:NH2	1:A:550:GLU:OE1	2.53	0.42
1:C:516:PHE:HZ	1:C:550:GLU:HG3	1.84	0.42
1:D:589:TRP:CG	1:D:590:LEU:H	2.37	0.42
1:C:463:VAL:HA	1:C:469:ILE:CD1	2.48	0.42
1:B:223:PHE:CZ	1:B:303:MET:HG3	2.55	0.42
1:D:132:LEU:CD1	1:D:590:LEU:CD2	2.97	0.42
1:C:7:ILE:HD13	1:C:358:LEU:HD11	2.01	0.42
1:C:186:LYS:NZ	2:C:642:HOH:O	2.52	0.42
1:A:63:MET:SD	1:A:65:MET:HG2	2.60	0.42
1:B:91:HIS:CE1	1:B:148:ALA:HB2	2.55	0.42
1:D:330:LYS:HD2	1:D:383:HIS:C	2.45	0.42
1:D:527:ILE:HG21	1:D:558:LYS:HB2	2.02	0.42
1:C:91:HIS:CE1	1:C:148:ALA:HB2	2.55	0.42
1:A:12:GLY:O	1:A:19:ASN:HA	2.20	0.42
1:A:58:VAL:HG12	1:A:208:MET:HE3	2.02	0.42
1:A:202:PRO:O	1:A:206:MET:CB	2.64	0.42
1:B:401:LYS:HA	1:B:401:LYS:HD2	1.94	0.42
1:C:542:THR:O	1:C:545:GLU:CG	2.68	0.42
1:B:443:VAL:HB	1:B:556:TRP:CH2	2.55	0.41
1:D:516:PHE:CD2	1:D:554:GLU:HG2	2.55	0.41
1:C:541:GLN:NE2	1:C:541:GLN:HA	2.35	0.41
1:B:18:ARG:HG3	2:B:617:HOH:O	2.19	0.41
1:B:308:THR:CG2	1:B:311:GLY:H	2.33	0.41
1:C:328:ASP:O	1:C:330:LYS:HE2	2.20	0.41
1:D:18:ARG:NH2	2:D:639:HOH:O	2.54	0.41
1:B:463:VAL:HA	1:B:469:ILE:HD12	2.02	0.41
1:C:285:ARG:HD3	1:C:325:GLU:OE2	2.20	0.41
1:C:332:PHE:CE2	1:C:385:PRO:HB3	2.54	0.41
1:A:181:GLN:OE1	1:A:181:GLN:HA	2.20	0.41
1:A:204:SER:O	1:A:206:MET:N	2.54	0.41
1:A:328:ASP:O	1:A:330:LYS:HE2	2.21	0.41
1:C:12:GLY:O	1:C:19:ASN:HA	2.21	0.41
1:A:521:LYS:HZ2	1:A:524:LYS:NZ	2.16	0.41
1:B:344:HIS:CD2	1:B:344:HIS:C	2.99	0.41
1:A:544:ILE:HG21	1:A:566:LYS:HB2	2.03	0.41
1:B:181:GLN:HG3	2:D:829:HOH:O	2.20	0.41
1:B:438:ARG:HA	1:B:438:ARG:HD2	1.90	0.41
1:B:547:LYS:O	1:B:547:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:HIS:CE1	1:D:148:ALA:HB2	2.56	0.41
1:B:524:LYS:O	1:B:528:LYS:HG3	2.21	0.41
1:D:346:SER:O	1:D:348:ALA:N	2.53	0.41
1:A:58:VAL:CB	1:A:208:MET:CE	2.99	0.40
1:C:3:ASP:O	2:C:606:HOH:O	2.22	0.40
1:A:203:GLU:O	1:A:206:MET:HB3	2.22	0.40
1:A:533:ASP:OD1	1:A:534:HIS:N	2.55	0.40
1:C:463:VAL:HA	1:C:469:ILE:HD12	2.03	0.40
1:A:3:ASP:N	2:A:650:HOH:O	2.54	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:636:HOH:O	2:A:679:HOH:O[2_745]	2.05	0.15
1:A:467:GLU:OE1	1:C:460:LYS:NZ[1_655]	2.08	0.12
2:B:899:HOH:O	2:D:889:HOH:O[1_455]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/617 (90%)	539 (98%)	13 (2%)	1 (0%)	43	42
1	B	560/617 (91%)	545 (97%)	15 (3%)	0	100	100
1	C	521/617 (84%)	510 (98%)	10 (2%)	1 (0%)	43	42
1	D	520/617 (84%)	504 (97%)	16 (3%)	0	100	100
All	All	2154/2468 (87%)	2098 (97%)	54 (2%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	TYR
1	C	544	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/515 (91%)	462 (99%)	6 (1%)	61	68
1	B	473/515 (92%)	461 (98%)	12 (2%)	42	45
1	C	442/515 (86%)	434 (98%)	8 (2%)	51	58
1	D	441/515 (86%)	426 (97%)	15 (3%)	32	33
All	All	1824/2060 (88%)	1783 (98%)	41 (2%)	45	50

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	LYS
1	A	439	SER
1	A	520	VAL
1	A	522	THR
1	A	527	ILE
1	A	554	GLU
1	B	20	VAL
1	B	58	VAL
1	B	272	ILE
1	B	308	THR
1	B	309	LYS
1	B	310	GLN
1	B	331	GLN
1	B	439	SER
1	B	455	TYR
1	B	512	ASN
1	B	520	VAL
1	B	529	LEU
1	C	20	VAL
1	C	399	ASP

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Mol	Chain	Res	Type
1	C	439	SER
1	C	520	VAL
1	C	522	THR
1	C	525	SER
1	C	545	GLU
1	C	546	LYS
1	D	20	VAL
1	D	317	GLU
1	D	396	GLU
1	D	401	LYS
1	D	455	TYR
1	D	504	ASP
1	D	520	VAL
1	D	521	LYS
1	D	524	LYS
1	D	526	GLU
1	D	528	LYS
1	D	529	LEU
1	D	531	GLU
1	D	537	LYS
1	D	561	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	344	HIS
1	A	416	ASN
1	B	126	ASN
1	B	270	ASN
1	B	344	HIS
1	B	378	HIS
1	B	383	HIS
1	B	416	ASN
1	C	91	HIS
1	C	331	GLN
1	C	416	ASN
1	C	534	HIS
1	D	96	GLN
1	D	126	ASN
1	D	416	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 [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, 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	563/617 (91%)	1.21	116 (20%) 2 2	23, 37, 68, 106	0
1	B	568/617 (92%)	1.24	116 (20%) 3 2	25, 39, 71, 109	0
1	C	533/617 (86%)	1.35	134 (25%) 1 1	24, 40, 76, 108	0
1	D	532/617 (86%)	1.47	133 (25%) 2 1	25, 39, 71, 106	0
All	All	2196/2468 (88%)	1.32	499 (22%) 2 2	23, 39, 73, 109	0

All (499) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	527	ILE	12.7
1	D	530	PHE	8.4
1	D	399	ASP	8.0
1	C	400	GLY	7.9
1	D	529	LEU	7.8
1	D	305	GLY	7.8
1	B	512	ASN	7.2
1	C	544	ILE	6.8
1	B	513	GLY	6.7
1	B	529	LEU	6.5
1	A	60	CYS	6.2
1	D	469	ILE	6.0
1	B	57	LYS	6.0
1	B	528	LYS	6.0
1	B	511	PRO	6.0
1	C	546	LYS	5.8
1	B	52	LEU	5.8
1	A	536	ALA	5.7
1	C	468	ASP	5.7
1	D	560	LEU	5.6
1	D	522	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	107	TYR	5.4
1	D	566	LYS	5.4
1	C	543	TRP	5.3
1	D	272	ILE	5.3
1	C	547	LYS	5.3
1	D	531	GLU	5.3
1	D	535	ASP	5.3
1	A	537	LYS	5.3
1	A	206	MET	5.1
1	D	398	ALA	5.1
1	C	132	LEU	5.1
1	D	523	LYS	5.0
1	D	526	GLU	4.9
1	A	47	TYR	4.9
1	A	547	LYS	4.9
1	C	535	ASP	4.8
1	C	305	GLY	4.8
1	C	20	VAL	4.8
1	B	330	LYS	4.8
1	B	142	GLY	4.8
1	B	51	VAL	4.8
1	B	514	SER	4.7
1	D	534	HIS	4.7
1	D	375	PRO	4.7
1	D	519	HIS	4.6
1	D	205	TYR	4.6
1	D	306	THR	4.6
1	B	510	MET	4.6
1	D	132	LEU	4.6
1	C	545	GLU	4.5
1	D	542	THR	4.5
1	D	528	LYS	4.5
1	D	37	ILE	4.5
1	B	308	THR	4.5
1	D	525	SER	4.4
1	A	217	ASP	4.4
1	A	208	MET	4.4
1	A	215	SER	4.4
1	C	527	ILE	4.4
1	B	375	PRO	4.4
1	A	310	GLN	4.4
1	A	229	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	534	HIS	4.4
1	B	228	ASN	4.4
1	A	544	ILE	4.4
1	C	532	THR	4.3
1	D	538	ALA	4.3
1	A	469	ILE	4.3
1	A	306	THR	4.3
1	B	141	THR	4.3
1	B	522	THR	4.3
1	D	3	ASP	4.3
1	D	400	GLY	4.3
1	C	306	THR	4.3
1	A	525	SER	4.3
1	D	141	THR	4.3
1	D	307	GLY	4.2
1	D	544	ILE	4.2
1	C	374	THR	4.2
1	C	464	THR	4.2
1	A	322	VAL	4.2
1	A	133	ASN	4.2
1	A	569	GLY	4.2
1	C	534	HIS	4.2
1	C	591	PRO	4.1
1	D	536	ALA	4.1
1	D	540	LEU	4.1
1	C	542	THR	4.1
1	B	520	VAL	4.1
1	A	538	ALA	4.1
1	B	272	ILE	4.1
1	A	205	TYR	4.0
1	D	571	TYR	4.0
1	A	542	THR	4.0
1	C	205	TYR	4.0
1	C	536	ALA	4.0
1	D	230	PHE	4.0
1	B	209	CYS	4.0
1	C	525	SER	3.9
1	A	511	PRO	3.9
1	C	504	ASP	3.9
1	A	522	THR	3.9
1	D	567	LEU	3.9
1	C	39	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	548	ARG	3.9
1	A	216	PRO	3.9
1	B	521	LYS	3.8
1	C	540	LEU	3.8
1	D	524	LYS	3.8
1	D	532	THR	3.8
1	C	530	PHE	3.8
1	A	539	LEU	3.8
1	A	375	PRO	3.8
1	A	207	SER	3.7
1	C	308	THR	3.7
1	D	309	LYS	3.7
1	B	58	VAL	3.7
1	A	520	VAL	3.7
1	A	59	TYR	3.7
1	C	3	ASP	3.7
1	D	382	GLU	3.7
1	C	567	LEU	3.7
1	A	510	MET	3.7
1	A	58	VAL	3.7
1	A	374	THR	3.7
1	A	543	TRP	3.6
1	D	42	TRP	3.6
1	A	514	SER	3.6
1	A	227	ALA	3.6
1	A	51	VAL	3.6
1	D	520	VAL	3.6
1	B	527	ILE	3.6
1	C	538	ALA	3.6
1	D	380	GLU	3.6
1	C	230	PHE	3.6
1	C	469	ILE	3.6
1	C	398	ALA	3.6
1	C	529	LEU	3.6
1	C	524	LYS	3.6
1	B	544	ILE	3.5
1	C	390	THR	3.5
1	D	464	THR	3.5
1	C	227	ALA	3.5
1	C	438	ARG	3.5
1	D	468	ASP	3.5
1	B	542	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	512	ASN	3.5
1	B	108	ASN	3.5
1	B	378	HIS	3.5
1	C	362	ASN	3.5
1	D	543	TRP	3.4
1	C	461	ASP	3.4
1	A	571	TYR	3.4
1	B	571	TYR	3.4
1	D	383	HIS	3.4
1	C	541	GLN	3.4
1	A	412	TYR	3.4
1	D	465	SER	3.4
1	D	537	LYS	3.4
1	D	547	LYS	3.4
1	A	549	LEU	3.4
1	B	59	TYR	3.3
1	B	400	GLY	3.3
1	D	40	SER	3.3
1	B	415	THR	3.3
1	D	204	SER	3.3
1	C	375	PRO	3.3
1	C	520	VAL	3.3
1	D	463	VAL	3.3
1	C	539	LEU	3.3
1	C	410	PHE	3.3
1	D	21	ARG	3.3
1	D	484	ALA	3.2
1	B	469	ILE	3.2
1	A	214	LEU	3.2
1	B	331	GLN	3.2
1	A	142	GLY	3.2
1	C	508	ALA	3.2
1	C	204	SER	3.2
1	D	374	THR	3.2
1	B	443	VAL	3.2
1	D	20	VAL	3.2
1	D	322	VAL	3.2
1	C	312	ASP	3.2
1	C	383	HIS	3.2
1	A	527	ILE	3.1
1	C	500	ILE	3.1
1	B	412	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	532	THR	3.1
1	C	229	GLY	3.1
1	D	313	PRO	3.1
1	B	6	ALA	3.1
1	B	399	ASP	3.1
1	D	548	ARG	3.1
1	A	545	GLU	3.1
1	D	439	SER	3.1
1	B	379	PHE	3.1
1	D	376	ASN	3.1
1	B	67	ASP	3.1
1	A	449	GLU	3.1
1	C	396	GLU	3.1
1	A	48	TYR	3.1
1	D	25	ASP	3.1
1	D	550	GLU	3.1
1	B	508	ALA	3.1
1	D	130	VAL	3.1
1	B	208	MET	3.1
1	B	543	TRP	3.0
1	A	305	GLY	3.0
1	D	308	THR	3.0
1	D	373	THR	3.0
1	D	410	PHE	3.0
1	D	328	ASP	3.0
1	C	130	VAL	3.0
1	A	546	LYS	3.0
1	A	590	LEU	3.0
1	A	307	GLY	3.0
1	B	497	GLU	3.0
1	B	50	PRO	3.0
1	A	3	ASP	3.0
1	C	107	TYR	3.0
1	A	230	PHE	3.0
1	D	498	MET	3.0
1	D	142	GLY	3.0
1	A	182	ALA	2.9
1	A	108	ASN	2.9
1	A	370	LEU	2.9
1	C	370	LEU	2.9
1	C	376	ASN	2.9
1	B	533	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	310	GLN	2.9
1	A	529	LEU	2.9
1	B	539	LEU	2.9
1	D	539	LEU	2.9
1	D	87	MET	2.9
1	B	317	GLU	2.9
1	A	372	PHE	2.9
1	B	107	TYR	2.9
1	B	538	ALA	2.9
1	B	532	THR	2.9
1	C	510	MET	2.9
1	A	50	PRO	2.9
1	B	130	VAL	2.8
1	B	449	GLU	2.8
1	A	36	ASP	2.8
1	B	536	ALA	2.8
1	A	220	CYS	2.8
1	B	44	VAL	2.8
1	B	60	CYS	2.8
1	A	309	LYS	2.8
1	D	541	GLN	2.8
1	A	400	GLY	2.8
1	D	569	GLY	2.8
1	A	380	GLU	2.8
1	C	317	GLU	2.8
1	B	268	LYS	2.8
1	D	184	ILE	2.8
1	B	525	SER	2.8
1	C	18	ARG	2.8
1	C	531	GLU	2.8
1	B	273	THR	2.8
1	D	591	PRO	2.8
1	D	193	VAL	2.8
1	B	20	VAL	2.7
1	D	470	ASP	2.7
1	B	496	ARG	2.7
1	C	385	PRO	2.7
1	D	108	ASN	2.7
1	B	213	MET	2.7
1	A	562	ILE	2.7
1	A	383	HIS	2.7
1	D	367	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	142	GLY	2.7
1	C	42	TRP	2.7
1	A	362	ASN	2.6
1	C	549	LEU	2.6
1	D	426	PRO	2.6
1	C	169	SER	2.6
1	D	461	ASP	2.6
1	D	504	ASP	2.6
1	A	287	ILE	2.6
1	C	226	GLY	2.6
1	B	42	TRP	2.6
1	B	65	MET	2.6
1	C	378	HIS	2.6
1	B	397	THR	2.6
1	A	524	LYS	2.6
1	C	384	SER	2.6
1	D	501	LYS	2.6
1	D	424	TYR	2.6
1	B	515	ILE	2.6
1	B	129	GLY	2.6
1	A	213	MET	2.6
1	C	466	ASN	2.6
1	A	551	LYS	2.6
1	C	81	PRO	2.6
1	A	468	ASP	2.6
1	A	204	SER	2.6
1	C	372	PHE	2.6
1	C	425	GLN	2.6
1	A	550	GLU	2.6
1	B	382	GLU	2.6
1	C	330	LYS	2.6
1	C	537	LYS	2.6
1	A	533	ASP	2.6
1	C	202	PRO	2.6
1	C	112	LEU	2.6
1	A	531	GLU	2.5
1	A	513	GLY	2.5
1	C	571	TYR	2.5
1	A	523	LYS	2.5
1	C	26	ASN	2.5
1	C	67	ASP	2.5
1	C	399	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	313	PRO	2.5
1	D	475	ALA	2.5
1	C	444	LEU	2.5
1	C	203	GLU	2.5
1	B	500	ILE	2.5
1	C	336	GLY	2.5
1	A	376	ASN	2.5
1	D	563	ASP	2.5
1	A	398	ALA	2.5
1	B	530	PHE	2.5
1	B	523	LYS	2.5
1	D	546	LYS	2.5
1	B	550	GLU	2.5
1	B	279	SER	2.5
1	D	39	THR	2.5
1	D	129	GLY	2.5
1	D	311	GLY	2.5
1	C	254	ILE	2.5
1	D	552	VAL	2.4
1	C	439	SER	2.4
1	D	74	PRO	2.4
1	A	222	ALA	2.4
1	C	517	ALA	2.4
1	A	567	LEU	2.4
1	B	278	LYS	2.4
1	B	383	HIS	2.4
1	D	229	GLY	2.4
1	A	298	ILE	2.4
1	A	333	CYS	2.4
1	D	60	CYS	2.4
1	B	38	PRO	2.4
1	D	381	PHE	2.4
1	C	533	ASP	2.4
1	A	272	ILE	2.4
1	D	568	TYR	2.4
1	D	347	ALA	2.4
1	D	553	ALA	2.4
1	B	471	LEU	2.4
1	B	492	LEU	2.4
1	C	27	LEU	2.4
1	C	590	LEU	2.4
1	A	83	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	212	GLY	2.4
1	B	231	VAL	2.4
1	B	547	LYS	2.4
1	C	276	SER	2.4
1	C	365	THR	2.4
1	C	412	TYR	2.3
1	A	540	LEU	2.3
1	B	549	LEU	2.3
1	C	200	LEU	2.3
1	C	311	GLY	2.3
1	D	12	GLY	2.3
1	B	461	ASP	2.3
1	A	186	LYS	2.3
1	B	465	SER	2.3
1	C	28	VAL	2.3
1	B	48	TYR	2.3
1	C	417	ALA	2.3
1	C	409	SER	2.3
1	D	562	ILE	2.3
1	C	511	PRO	2.3
1	A	42	TRP	2.3
1	A	548	ARG	2.3
1	C	486	ASP	2.3
1	D	533	ASP	2.3
1	B	309	LYS	2.3
1	A	40	SER	2.3
1	C	381	PHE	2.3
1	D	114	GLU	2.3
1	B	562	ILE	2.3
1	C	188	ILE	2.3
1	A	373	THR	2.3
1	C	369	THR	2.3
1	A	109	ALA	2.3
1	B	328	ASP	2.3
1	B	398	ALA	2.3
1	C	501	LYS	2.3
1	C	566	LYS	2.3
1	D	227	ALA	2.3
1	B	178	LEU	2.3
1	B	567	LEU	2.3
1	B	14	TYR	2.3
1	B	169	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	273	THR	2.2
1	B	201	THR	2.2
1	D	401	LYS	2.2
1	C	43	ASP	2.2
1	C	266	ASP	2.2
1	C	274	ALA	2.2
1	C	502	ALA	2.2
1	C	569	GLY	2.2
1	B	366	LEU	2.2
1	B	540	LEU	2.2
1	B	85	GLU	2.2
1	B	487	TYR	2.2
1	B	570	GLU	2.2
1	C	199	TYR	2.2
1	B	306	THR	2.2
1	D	443	VAL	2.2
1	B	585	GLU	2.2
1	D	584	ALA	2.2
1	A	492	LEU	2.2
1	B	541	GLN	2.2
1	D	412	TYR	2.2
1	D	79	ILE	2.2
1	B	322	VAL	2.2
1	D	226	GLY	2.2
1	D	316	LEU	2.2
1	B	61	LYS	2.2
1	C	528	LYS	2.2
1	A	228	ASN	2.2
1	A	589	TRP	2.2
1	A	308	THR	2.2
1	C	377	GLU	2.1
1	D	379	PHE	2.1
1	C	324	GLN	2.1
1	D	508	ALA	2.1
1	D	549	LEU	2.1
1	D	495	SER	2.1
1	C	63	MET	2.1
1	C	389	ASN	2.1
1	D	107	TYR	2.1
1	D	83	GLU	2.1
1	D	449	GLU	2.1
1	A	500	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	257	ILE	2.1
1	C	314	ILE	2.1
1	A	226	GLY	2.1
1	C	388	VAL	2.1
1	D	378	HIS	2.1
1	C	62	SER	2.1
1	D	492	LEU	2.1
1	B	376	ASN	2.1
1	D	362	ASN	2.1
1	D	510	MET	2.1
1	D	487	TYR	2.1
1	A	202	PRO	2.1
1	A	269	THR	2.1
1	A	295	PRO	2.1
1	B	591	PRO	2.1
1	C	426	PRO	2.1
1	D	511	PRO	2.1
1	A	271	GLY	2.1
1	B	184	ILE	2.1
1	B	438	ARG	2.1
1	C	21	ARG	2.1
1	D	351	VAL	2.1
1	A	211	ALA	2.1
1	A	247	ALA	2.1
1	C	454	ALA	2.1
1	C	580	ALA	2.1
1	D	440	ALA	2.1
1	C	340	SER	2.1
1	A	470	ASP	2.1
1	A	74	PRO	2.1
1	B	373	THR	2.1
1	B	534	HIS	2.1
1	C	401	LYS	2.1
1	C	523	LYS	2.1
1	A	381	PHE	2.1
1	B	516	PHE	2.1
1	D	231	VAL	2.1
1	C	553	ALA	2.1
1	C	131	MET	2.0
1	C	366	LEU	2.0
1	C	492	LEU	2.0
1	D	198	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	219	GLN	2.0
1	C	333	CYS	2.0
1	D	496	ARG	2.0
1	A	528	LYS	2.0
1	B	428	LYS	2.0
1	C	521	LYS	2.0
1	D	491	PHE	2.0
1	D	62	SER	2.0
1	B	24	TRP	2.0
1	B	362	ASN	2.0
1	A	316	LEU	2.0
1	B	504	ASP	2.0
1	A	115	LYS	2.0
1	B	524	LYS	2.0
1	C	568	TYR	2.0
1	D	588	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.