



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 09:17 am GMT

PDB ID : 5E5N
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

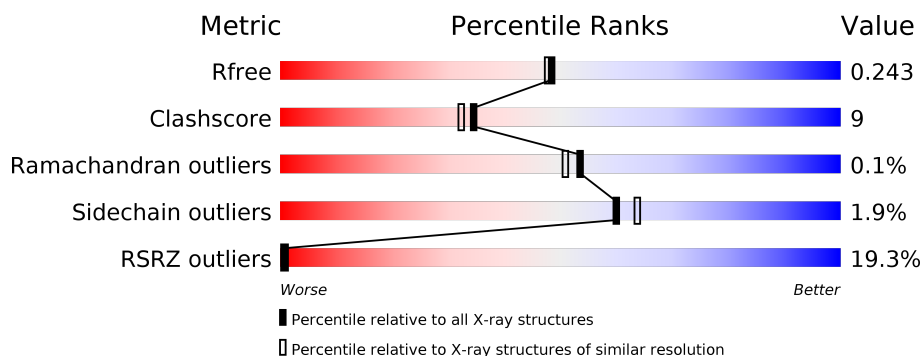
1 Overall quality at a glance

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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>18%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>9%</div> </div> </div>
1	B	617	<div> <div>17%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>
1	C	617	<div> <div>16%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>14%</div> </div> </div>
1	D	617	<div> <div>18%</div> <div> <div></div> <div>74%</div> <div>11%</div> <div>14%</div> </div> </div>

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

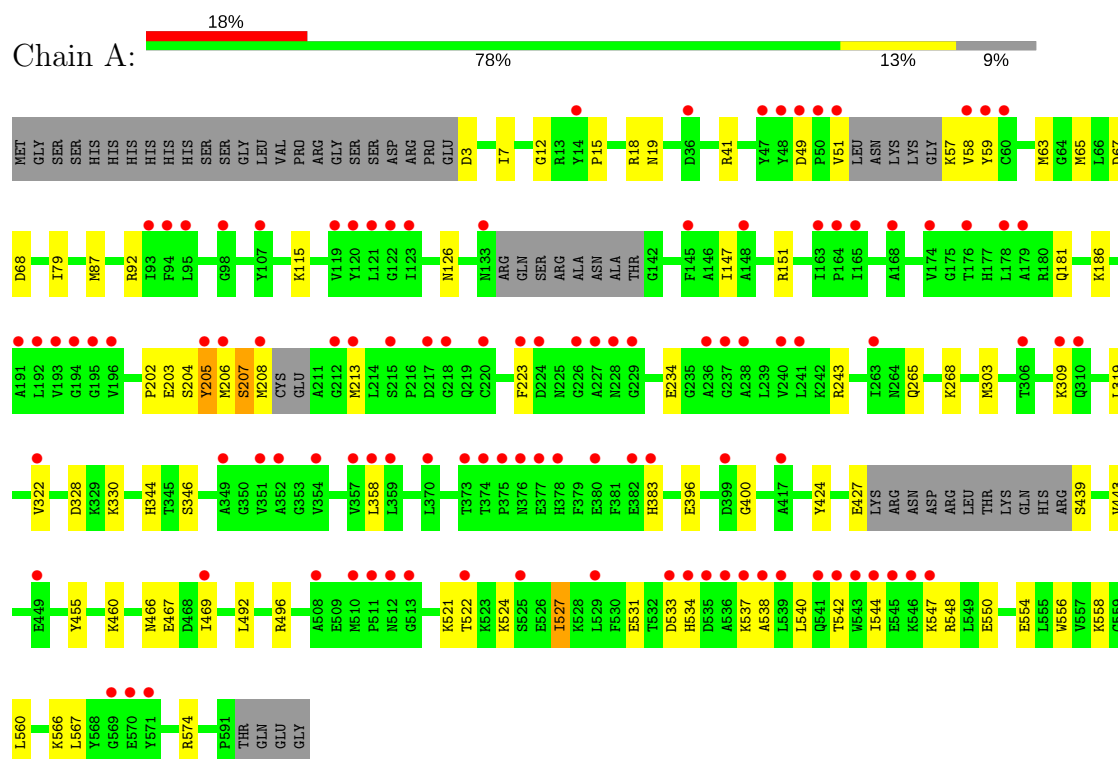
- Molecule 2 is water.

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		

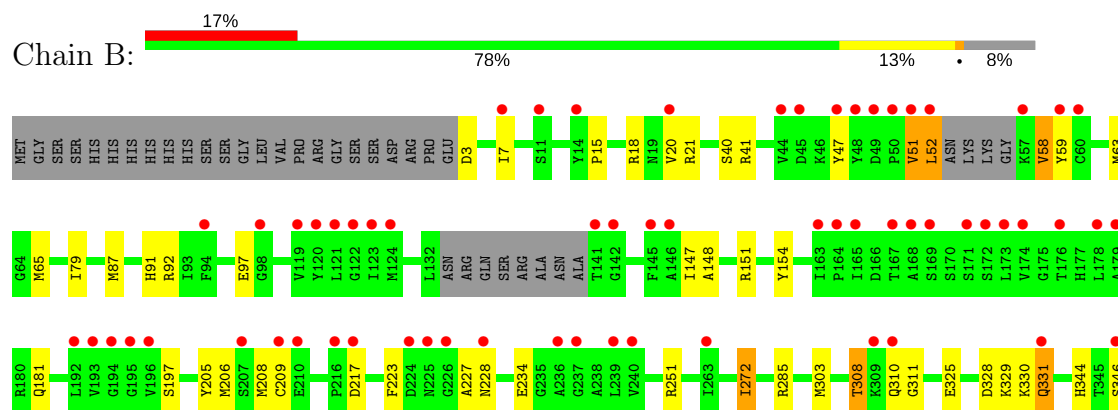
3 Residue-property plots [i](#)

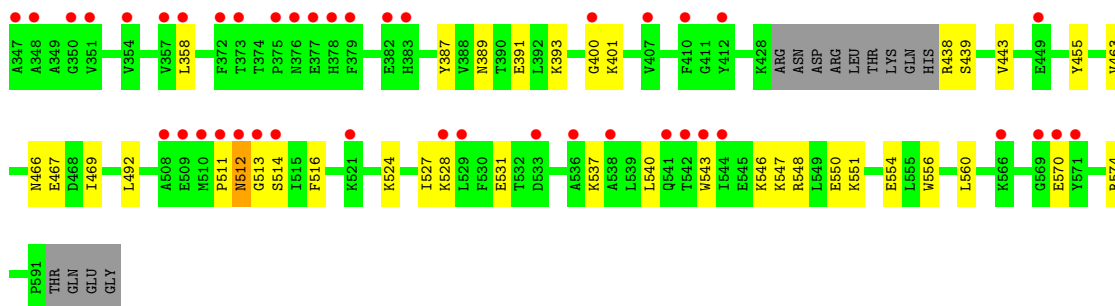
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Polyketide synthase PksL

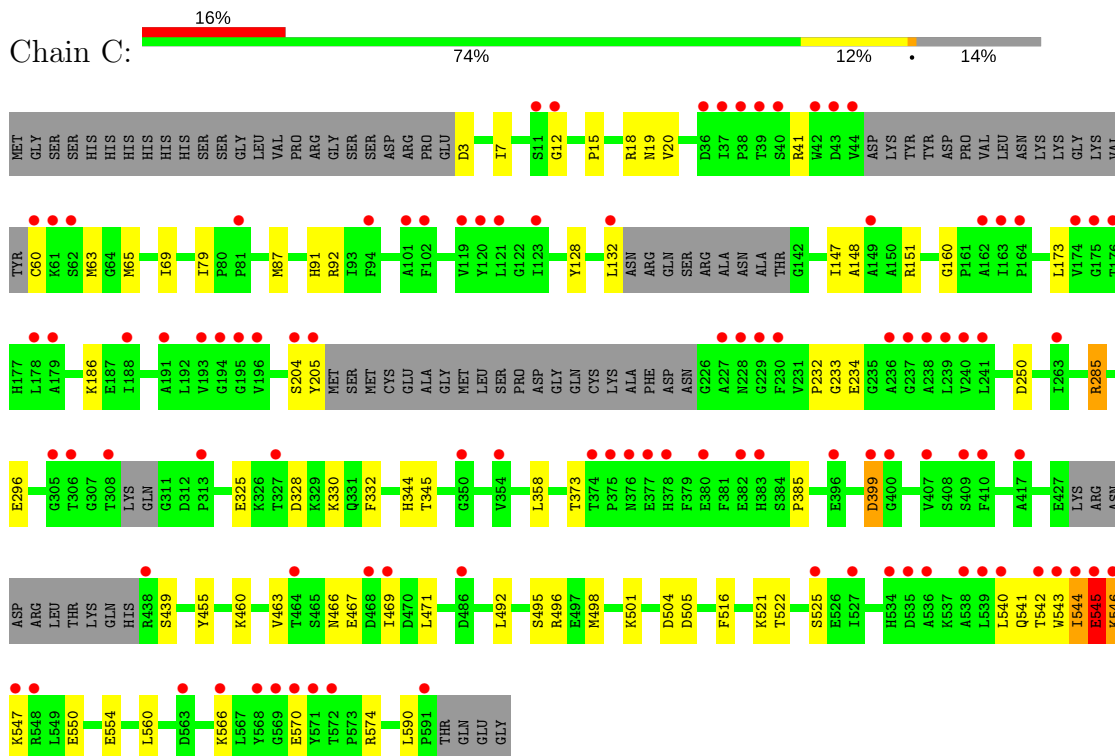


• Molecule 1: Polyketide synthase PksL

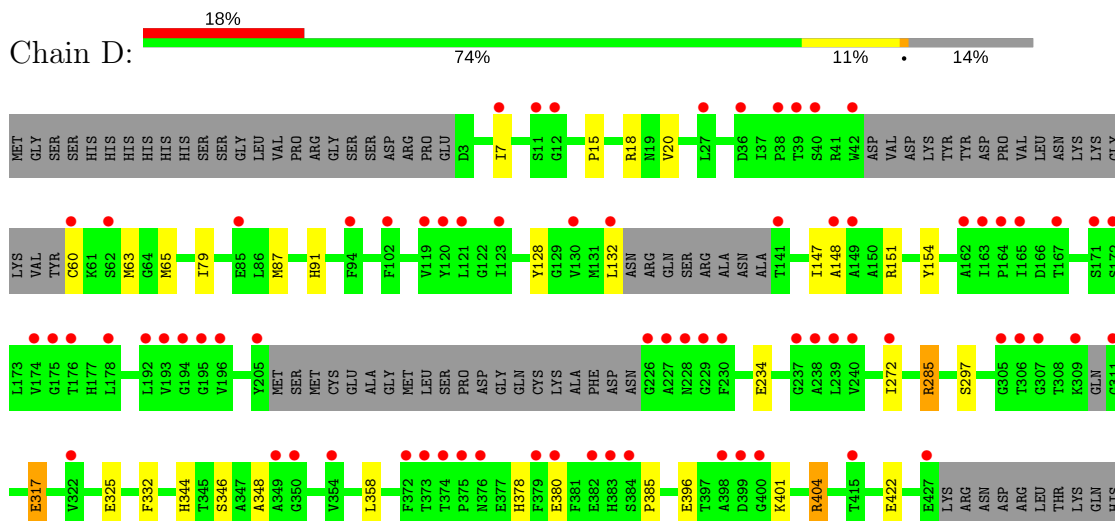


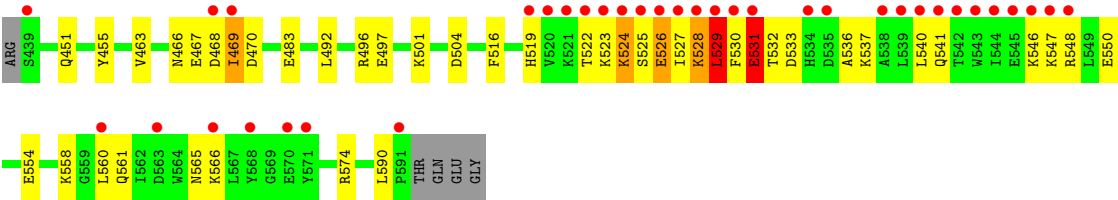


- Molecule 1: Polyketide synthase PksL



- 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 44.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (150.00-2.00) 99.2 (44.92-2.00)	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 (5.04%)	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 , 52.4	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	0.94	0/4518	0.72	2/6110 (0.0%)
1	B	0.93	2/4561 (0.0%)	0.79	7/6168 (0.1%)
1	C	0.90	0/4277	0.71	7/5784 (0.1%)
1	D	0.98	6/4266 (0.1%)	0.77	10/5768 (0.2%)
All	All	0.94	8/17622 (0.0%)	0.75	26/23830 (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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	531	GLU	CG-CD	-6.28	1.42	1.51
1	D	525	SER	CB-OG	6.25	1.50	1.42
1	D	297	SER	CB-OG	6.19	1.50	1.42
1	B	97	GLU	CD-OE1	5.93	1.32	1.25
1	D	404	ARG	CD-NE	-5.65	1.36	1.46
1	D	526	GLU	CD-OE2	5.61	1.31	1.25
1	D	531	GLU	C-O	5.55	1.33	1.23
1	B	197	SER	CB-OG	5.12	1.49	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	VAL	CB-CA-C	-18.49	76.28	111.40
1	B	514	SER	N-CA-CB	-14.74	88.39	110.50
1	B	52	LEU	N-CA-CB	-12.88	84.65	110.40
1	D	404	ARG	NE-CZ-NH2	12.12	126.36	120.30
1	D	529	LEU	CB-CA-C	-10.67	89.92	110.20
1	D	404	ARG	NE-CZ-NH1	-10.45	115.07	120.30
1	C	545	GLU	CB-CA-C	-9.36	91.69	110.40
1	D	531	GLU	CB-CA-C	8.92	128.24	110.40
1	B	513	GLY	N-CA-C	8.25	133.73	113.10
1	B	512	ASN	N-CA-CB	-7.81	96.53	110.60
1	C	545	GLU	N-CA-C	7.28	130.66	111.00
1	A	207	SER	N-CA-CB	6.96	120.94	110.50
1	D	404	ARG	CB-CG-CD	6.90	129.53	111.60
1	D	529	LEU	N-CA-C	6.82	129.40	111.00
1	B	41	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	B	511	PRO	CB-CA-C	-6.24	96.39	112.00
1	C	285	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	C	547	LYS	N-CA-C	6.01	127.24	111.00
1	A	41	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	D	285	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	469	ILE	CB-CA-C	-5.64	100.32	111.60
1	C	546	LYS	CB-CA-C	-5.53	99.34	110.40
1	D	285	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	D	531	GLU	N-CA-C	-5.31	96.66	111.00
1	C	18	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	C	399	ASP	CB-CA-C	-5.10	100.21	110.40

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	83	1
1	B	4461	0	4373	74	0
1	C	4185	0	4102	71	1
1	D	4174	0	4092	90	0
2	A	371	0	0	18	1
2	B	333	0	0	15	1
2	C	320	0	0	20	0
2	D	334	0	0	14	1
All	All	18597	0	16890	308	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 (308) 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:C:542:THR:O	2:C:601:HOH:O	1.55	1.19
1:B:467:GLU:CD	2:B:601:HOH:O	1.81	1.18
1:D:528:LYS:O	1:D:531:GLU:HB3	1.51	1.09
1:D:529:LEU:CD1	1:D:529:LEU:O	2.03	1.07
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:18:ARG:NH2	2:A:602:HOH:O	2.02	0.93
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: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: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:531:GLU:C	1:D:537:LYS:HZ3	1.75	0.88
1:D:529:LEU:HD12	1:D:529:LEU:O	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:58:VAL:HB	1:A:208:MET:HE3	1.57	0.86

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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:HD13	1:D:529:LEU:O	1.76	0.83
1:A:396:GLU:OE2	2:A:601:HOH:O	1.96	0.83
1:A:18:ARG:CZ	2:A:602:HOH:O	2.27	0.82
1:A:208:MET:C	1:A:213:MET:H	1.83	0.81
1:C:541:GLN:O	1:C:545:GLU:HG2	1.81	0.81
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:531:GLU:C	1:D:537:LYS:NZ	2.34	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:B:467:GLU:CG	2:B:601:HOH:O	2.28	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: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: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:D:79:ILE:HD13	1:D:87:MET:HE1	1.70	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:A:466:ASN:HB2	1:A:469:ILE:HD11	1.73	0.70
1:A:79:ILE:HD13	1:A:87:MET:HE1	1.72	0.70
1:C:542:THR:C	2:C:601:HOH:O	2.09	0.69
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:A:58:VAL:CB	1:A:208:MET:HE3	2.23	0.68
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:C:543:TRP:C	1:C:545:GLU:H	1.98	0.67
1:A:460:LYS:NZ	2:A:611:HOH:O	2.27	0.66
1:C:79:ILE:HD13	1:C:87:MET:HE1	1.77	0.66
1:A:521:LYS:HZ1	1:A:524:LYS:NZ	1.93	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: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: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:527:ILE:CD1	1:A:558:LYS:HB3	2.26	0.65
1:A:67:ASP:OD1	2:A:607:HOH:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	1:B:546:LYS:CD	2.48	0.61
1:B:47:TYR:CD1	1:B:206:MET:CE	2.84	0.61
1:B:79:ILE:HD13	1:B:87:MET:HE1	1.82	0.61
1:B:546:LYS:O	1:B:546:LYS:HD2	2.00	0.61
1:A:540:LEU:HD22	1:A:560:LEU:HD21	1.81	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:A:521:LYS:HZ1	1:A:524:LYS:HZ1	1.49	0.59
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:B:3:ASP:N	2:B:613:HOH:O	2.36	0.59
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:543:TRP:C	1:C:545:GLU:N	2.57	0.57
1:A:460:LYS:CE	2:A:611:HOH:O	2.52	0.57
1:A:521:LYS:NZ	1:A:524:LYS:HZ3	2.01	0.57
1:D:529:LEU:C	1:D:531:GLU:H	2.08	0.57
1:A:547:LYS:HE3	1:A:567:LEU:C	2.24	0.56
1:B:51:VAL:HG12	1:B:52:LEU:N	2.19	0.56
1:B:391:GLU:HG3	1:B:393:LYS:HD3	1.88	0.56
1:A:205:TYR:C	1:A:205:TYR:CD1	2.78	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:519:HIS:O	1:D:522:THR:OG1	2.19	0.55
1:D:497:GLU:CG	1:D:501:LYS:HE2	2.36	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:492:LEU:N	1:C:492:LEU:HD12	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:A:208:MET:C	1:A:213:MET:N	2.60	0.53
1:B:79:ILE:HD13	1:B:87:MET:CE	2.38	0.53
1:C:544:ILE:O	1:C:544:ILE:HG22	2.09	0.53
1:D:523:LYS:HD2	1:D:558:LYS:HG2	1.91	0.53
1:A:79:ILE:HD13	1:A:87:MET:CE	2.38	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:C:79:ILE:HD13	1:C:87:MET:CE	2.40	0.51
1:D:380:GLU:OE1	1:D:380:GLU:N	2.41	0.50
1:D:79:ILE:HD13	1:D:87:MET:CE	2.39	0.50
1:A:206:MET:O	1:A:208:MET:N	2.44	0.50
1:B:272:ILE:HG13	1:B:272:ILE:O	2.12	0.50
1:B:40:SER:OG	1:C:328:ASP:OD1	2.14	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:A:521:LYS:HZ2	1:A:524:LYS:NZ	2.08	0.49
1:C:542:THR:CA	1:C:545:GLU:HG3	2.39	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: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:D:380:GLU:CD	1:D:380:GLU:H	2.16	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:B:329:LYS:HG2	2:B:602:HOH:O	2.14	0.47
1:D:128:TYR:CD2	1:D:132:LEU:CD1	2.96	0.47
1:D:63:MET:SD	1:D:65:MET:HG2	2.55	0.47
1:A:265:GLN:HB2	1:C:160:GLY:O	2.14	0.47
1:B:79:ILE:HG21	1:B:87:MET:HE3	1.95	0.47
1:D:492:LEU:HD12	1:D:492:LEU:N	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: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:A:58:VAL:HA	1:A:208:MET:CE	2.46	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:268:LYS:NZ	2:A:628:HOH:O	2.46	0.44
1:A:521:LYS:NZ	1:A:524:LYS:HZ1	2.09	0.44
1:B:208:MET:HE3	2:B:917:HOH:O	2.17	0.44
1:A:521:LYS:HZ2	1:A:524:LYS:HZ3	1.63	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:463:VAL:HA	1:B:469:ILE:CD1	2.49	0.43
1:A:531:GLU:C	1:A:537:LYS:HE3	2.39	0.43
1:B:147:ILE:O	1:B:151:ARG:HG2	2.18	0.43
1:B:7:ILE:HD13	1:B:358:LEU:HD11	2.01	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:CD1	1:D:590:LEU:CD2	2.97	0.42
1:C:186:LYS:NZ	2:C:642:HOH:O	2.52	0.42
1:C:7:ILE:HD13	1:C:358:LEU:HD11	2.01	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:527:ILE:HG21	1:D:558:LYS:HB2	2.02	0.42
1:A:204:SER:C	1:A:206:MET:N	2.73	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: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:204:SER:O	1:A:205:TYR:C	2.59	0.41
1:D:469:ILE:HG22	1:D:470:ASP:C	2.41	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:D:91:HIS:CE1	1:D:148:ALA:HB2	2.56	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
1:B:570:GLU:CD	1:B:570:GLU:H	2.24	0.41
1:C:471:LEU:HD11	1:C:495:SER:C	2.40	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:206:MET:O	1:A:207:SER:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	49	46
1	B	560/617 (91%)	545 (97%)	15 (3%)	0	100	100
1	C	521/617 (84%)	510 (98%)	10 (2%)	1 (0%)	49	46
1	D	520/617 (84%)	504 (97%)	16 (3%)	0	100	100
All	All	2154/2468 (87%)	2098 (97%)	54 (2%)	2 (0%)	53	51

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%)	463 (99%)	5 (1%)	76	80
1	B	473/515 (92%)	465 (98%)	8 (2%)	63	68
1	C	442/515 (86%)	434 (98%)	8 (2%)	62	66
1	D	441/515 (86%)	428 (97%)	13 (3%)	45	45
All	All	1824/2060 (88%)	1790 (98%)	34 (2%)	60	64

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	LYS
1	A	439	SER
1	A	455	TYR
1	A	522	THR
1	A	527	ILE
1	B	20	VAL
1	B	58	VAL
1	B	272	ILE
1	B	308	THR
1	B	331	GLN
1	B	439	SER
1	B	455	TYR
1	B	512	ASN
1	C	20	VAL
1	C	399	ASP
1	C	439	SER
1	C	455	TYR
1	C	504	ASP
1	C	522	THR
1	C	525	SER
1	C	545	GLU
1	D	20	VAL
1	D	317	GLU
1	D	344	HIS

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Mol	Chain	Res	Type
1	D	396	GLU
1	D	401	LYS
1	D	455	TYR
1	D	504	ASP
1	D	524	LYS
1	D	526	GLU
1	D	528	LYS
1	D	529	LEU
1	D	531	GLU
1	D	561	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	HIS
1	B	270	ASN
1	B	344	HIS
1	B	378	HIS
1	C	541	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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%)	0.90	108 (19%) 1 1	23, 37, 68, 106	0
1	B	568/617 (92%)	0.89	105 (18%) 1 1	25, 39, 71, 109	0
1	C	533/617 (86%)	0.90	100 (18%) 1 1	24, 40, 76, 108	0
1	D	532/617 (86%)	1.02	110 (20%) 1 0	25, 39, 71, 106	0
All	All	2196/2468 (88%)	0.93	423 (19%) 1 1	23, 39, 73, 109	0

All (423) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	527	ILE	12.5
1	B	511	PRO	9.3
1	D	535	ASP	8.0
1	D	571	TYR	7.9
1	A	374	THR	7.6
1	C	44	VAL	7.3
1	C	400	GLY	7.2
1	B	512	ASN	7.1
1	A	536	ALA	7.1
1	D	399	ASP	6.9
1	D	400	GLY	6.7
1	A	310	GLN	6.5
1	D	522	THR	6.3
1	C	43	ASP	6.2
1	D	163	ILE	6.1
1	D	529	LEU	6.1
1	C	534	HIS	6.1
1	B	513	GLY	6.0
1	C	39	THR	6.0
1	D	40	SER	6.0
1	C	546	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	535	ASP	5.8
1	A	511	PRO	5.7
1	D	530	PHE	5.7
1	B	529	LEU	5.6
1	A	538	ALA	5.6
1	C	374	THR	5.5
1	A	547	LYS	5.4
1	A	510	MET	5.4
1	C	40	SER	5.3
1	D	42	TRP	5.3
1	C	132	LEU	5.3
1	D	205	TYR	5.3
1	D	523	LYS	5.3
1	A	544	ILE	5.2
1	A	534	HIS	5.2
1	D	519	HIS	5.2
1	B	510	MET	5.2
1	D	524	LYS	5.2
1	B	50	PRO	5.1
1	B	51	VAL	5.1
1	C	468	ASP	5.1
1	D	543	TRP	5.1
1	C	378	HIS	5.1
1	A	373	THR	5.1
1	C	174	VAL	4.9
1	D	375	PRO	4.9
1	A	48	TYR	4.9
1	A	163	ILE	4.9
1	C	544	ILE	4.9
1	D	531	GLU	4.9
1	D	374	THR	4.9
1	C	375	PRO	4.8
1	D	373	THR	4.8
1	B	174	VAL	4.8
1	C	438	ARG	4.8
1	C	538	ALA	4.8
1	B	178	LEU	4.8
1	A	47	TYR	4.7
1	D	272	ILE	4.7
1	A	60	CYS	4.7
1	D	39	THR	4.7
1	D	538	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	174	VAL	4.7
1	D	60	CYS	4.6
1	D	526	GLU	4.6
1	C	163	ILE	4.6
1	C	571	TYR	4.6
1	B	509	GLU	4.5
1	A	217	ASP	4.5
1	C	542	THR	4.5
1	D	238	ALA	4.5
1	A	226	GLY	4.4
1	A	193	VAL	4.4
1	D	547	LYS	4.4
1	A	380	GLU	4.4
1	B	165	ILE	4.4
1	B	48	TYR	4.4
1	D	528	LYS	4.3
1	B	351	VAL	4.3
1	A	59	TYR	4.3
1	C	42	TRP	4.3
1	B	173	LEU	4.2
1	D	398	ALA	4.2
1	D	544	ILE	4.2
1	D	165	ILE	4.2
1	C	383	HIS	4.2
1	B	52	LEU	4.2
1	A	383	HIS	4.2
1	A	375	PRO	4.1
1	A	178	LEU	4.1
1	B	44	VAL	4.1
1	C	547	LYS	4.1
1	C	205	TYR	4.1
1	B	163	ILE	4.1
1	B	536	ALA	4.1
1	A	571	TYR	4.0
1	D	520	VAL	4.0
1	B	310	GLN	4.0
1	B	528	LYS	4.0
1	A	229	GLY	4.0
1	D	123	ILE	4.0
1	B	375	PRO	3.9
1	B	521	LYS	3.9
1	C	238	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	193	VAL	3.9
1	D	176	THR	3.9
1	D	38	PRO	3.9
1	D	132	LEU	3.9
1	C	228	ASN	3.9
1	A	215	SER	3.9
1	B	192	LEU	3.9
1	D	119	VAL	3.9
1	D	307	GLY	3.9
1	A	569	GLY	3.8
1	B	194	GLY	3.8
1	D	237	GLY	3.8
1	B	196	VAL	3.8
1	B	382	GLU	3.8
1	B	571	TYR	3.8
1	D	195	GLY	3.8
1	A	513	GLY	3.7
1	C	229	GLY	3.7
1	B	377	GLU	3.7
1	B	383	HIS	3.7
1	D	194	GLY	3.7
1	B	168	ALA	3.7
1	D	141	THR	3.7
1	C	196	VAL	3.7
1	A	196	VAL	3.7
1	B	119	VAL	3.7
1	B	239	LEU	3.6
1	B	122	GLY	3.6
1	B	228	ASN	3.6
1	B	195	GLY	3.6
1	D	566	LYS	3.6
1	D	591	PRO	3.6
1	B	121	LEU	3.6
1	A	205	TYR	3.6
1	C	399	ASP	3.6
1	B	544	ILE	3.5
1	A	376	ASN	3.5
1	D	534	HIS	3.5
1	A	570	GLU	3.5
1	D	469	ILE	3.5
1	A	50	PRO	3.5
1	C	570	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	164	PRO	3.5
1	C	60	CYS	3.5
1	C	195	GLY	3.5
1	D	540	LEU	3.5
1	B	59	TYR	3.5
1	D	380	GLU	3.5
1	B	378	HIS	3.5
1	A	208	MET	3.5
1	D	525	SER	3.5
1	A	378	HIS	3.5
1	B	263	ILE	3.5
1	B	508	ALA	3.5
1	A	218	GLY	3.4
1	B	543	TRP	3.4
1	A	240	VAL	3.4
1	D	174	VAL	3.4
1	D	350	GLY	3.4
1	A	537	LYS	3.4
1	C	572	THR	3.4
1	B	237	GLY	3.4
1	C	545	GLU	3.4
1	C	569	GLY	3.4
1	A	228	ASN	3.4
1	D	545	GLU	3.3
1	A	123	ILE	3.3
1	C	237	GLY	3.3
1	D	229	GLY	3.3
1	C	527	ILE	3.3
1	B	570	GLU	3.3
1	A	192	LEU	3.3
1	B	123	ILE	3.3
1	B	373	THR	3.3
1	B	514	SER	3.3
1	C	121	LEU	3.3
1	D	539	LEU	3.2
1	A	194	GLY	3.2
1	A	133	ASN	3.2
1	A	309	LYS	3.2
1	C	591	PRO	3.2
1	A	121	LEU	3.2
1	B	354	VAL	3.2
1	D	548	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	525	SER	3.2
1	D	560	LEU	3.2
1	C	548	ARG	3.2
1	B	94	PHE	3.2
1	B	449	GLU	3.1
1	C	380	GLU	3.1
1	B	376	ASN	3.1
1	A	107	TYR	3.1
1	A	241	LEU	3.1
1	D	239	LEU	3.1
1	D	521	LYS	3.1
1	A	168	ALA	3.1
1	D	149	ALA	3.1
1	A	224	ASP	3.1
1	A	352	ALA	3.1
1	D	382	GLU	3.1
1	D	148	ALA	3.1
1	A	449	GLU	3.1
1	D	12	GLY	3.1
1	C	540	LEU	3.1
1	C	407	VAL	3.1
1	D	196	VAL	3.1
1	A	176	THR	3.1
1	C	176	THR	3.1
1	B	14	TYR	3.1
1	A	195	GLY	3.0
1	D	383	HIS	3.0
1	A	542	THR	3.0
1	C	396	GLU	3.0
1	A	119	VAL	3.0
1	A	191	ALA	3.0
1	C	539	LEU	3.0
1	A	51	VAL	3.0
1	D	354	VAL	3.0
1	B	47	TYR	3.0
1	B	120	TYR	3.0
1	C	178	LEU	3.0
1	A	227	ALA	3.0
1	D	193	VAL	3.0
1	C	120	TYR	3.0
1	C	377	GLU	3.0
1	B	57	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	427	GLU	3.0
1	C	469	ILE	3.0
1	D	230	PHE	3.0
1	B	209	CYS	2.9
1	C	464	THR	2.9
1	A	164	PRO	2.9
1	D	121	LEU	2.9
1	D	192	LEU	2.9
1	C	164	PRO	2.9
1	C	204	SER	2.9
1	D	162	ALA	2.9
1	B	169	SER	2.9
1	C	543	TRP	2.9
1	B	357	VAL	2.8
1	C	308	THR	2.8
1	B	145	PHE	2.8
1	C	566	LYS	2.8
1	D	306	THR	2.8
1	B	542	THR	2.8
1	A	120	TYR	2.8
1	B	172	SER	2.8
1	C	417	ALA	2.8
1	A	508	ALA	2.7
1	B	538	ALA	2.7
1	C	149	ALA	2.7
1	D	36	ASP	2.7
1	B	49	ASP	2.7
1	B	236	ALA	2.7
1	D	311	GLY	2.7
1	C	191	ALA	2.7
1	C	240	VAL	2.7
1	B	379	PHE	2.7
1	D	309	LYS	2.7
1	A	539	LEU	2.7
1	C	241	LEU	2.7
1	B	60	CYS	2.7
1	D	541	GLN	2.7
1	A	145	PHE	2.7
1	A	529	LEU	2.7
1	C	376	ASN	2.7
1	D	570	GLU	2.6
1	A	546	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	305	GLY	2.6
1	C	61	LYS	2.6
1	B	7	ILE	2.6
1	C	162	ALA	2.6
1	C	525	SER	2.6
1	A	263	ILE	2.6
1	B	146	ALA	2.6
1	A	469	ILE	2.6
1	C	123	ILE	2.6
1	D	178	LEU	2.6
1	B	309	LYS	2.6
1	B	348	ALA	2.6
1	D	226	GLY	2.6
1	A	322	VAL	2.5
1	C	119	VAL	2.5
1	B	346	SER	2.5
1	A	36	ASP	2.5
1	C	62	SER	2.5
1	C	193	VAL	2.5
1	D	563	ASP	2.5
1	C	350	GLY	2.5
1	C	354	VAL	2.5
1	A	382	GLU	2.5
1	B	171	SER	2.5
1	C	409	SER	2.5
1	D	439	SER	2.5
1	A	512	ASN	2.5
1	C	175	GLY	2.5
1	A	236	ALA	2.5
1	C	179	ALA	2.5
1	C	568	TYR	2.5
1	B	164	PRO	2.5
1	A	220	CYS	2.5
1	D	172	SER	2.5
1	D	376	ASN	2.5
1	C	230	PHE	2.5
1	D	94	PHE	2.5
1	A	206	MET	2.4
1	A	351	VAL	2.4
1	C	236	ALA	2.4
1	D	227	ALA	2.4
1	D	372	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	533	ASP	2.4
1	B	240	VAL	2.4
1	A	165	ILE	2.4
1	C	536	ALA	2.4
1	A	223	PHE	2.4
1	C	37	ILE	2.4
1	A	358	LEU	2.4
1	B	358	LEU	2.4
1	C	194	GLY	2.4
1	B	124	MET	2.4
1	A	545	GLU	2.4
1	C	313	PRO	2.4
1	A	349	ALA	2.4
1	B	372	PHE	2.3
1	C	94	PHE	2.3
1	D	171	SER	2.3
1	B	167	THR	2.3
1	B	331	GLN	2.3
1	D	568	TYR	2.3
1	C	38	PRO	2.3
1	C	239	LEU	2.3
1	A	357	VAL	2.3
1	B	20	VAL	2.3
1	B	179	ALA	2.3
1	C	227	ALA	2.3
1	C	382	GLU	2.3
1	B	216	PRO	2.3
1	B	11	SER	2.3
1	C	305	GLY	2.3
1	A	58	VAL	2.3
1	A	354	VAL	2.3
1	A	522	THR	2.3
1	D	542	THR	2.3
1	B	142	GLY	2.3
1	D	62	SER	2.3
1	C	101	ALA	2.3
1	D	379	PHE	2.3
1	B	141	THR	2.3
1	B	176	THR	2.3
1	A	212	GLY	2.3
1	A	237	GLY	2.3
1	B	225	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	228	ASN	2.3
1	C	263	ILE	2.3
1	A	179	ALA	2.2
1	A	359	LEU	2.2
1	B	407	VAL	2.2
1	A	543	TRP	2.2
1	A	14	TYR	2.2
1	B	412	TYR	2.2
1	A	94	PHE	2.2
1	B	98	GLY	2.2
1	B	224	ASP	2.2
1	A	377	GLU	2.2
1	A	122	GLY	2.2
1	D	468	ASP	2.2
1	D	546	LYS	2.2
1	A	95	LEU	2.2
1	B	350	GLY	2.2
1	C	12	GLY	2.2
1	A	49	ASP	2.2
1	C	102	PHE	2.2
1	C	563	ASP	2.2
1	D	102	PHE	2.2
1	A	399	ASP	2.2
1	D	11	SER	2.2
1	D	240	VAL	2.2
1	B	45	ASP	2.2
1	C	36	ASP	2.2
1	D	175	GLY	2.2
1	D	27	LEU	2.1
1	A	306	THR	2.1
1	B	347	ALA	2.1
1	C	188	ILE	2.1
1	B	541	GLN	2.1
1	D	120	TYR	2.1
1	D	384	SER	2.1
1	D	85	GLU	2.1
1	C	486	ASP	2.1
1	D	130	VAL	2.1
1	D	322	VAL	2.1
1	A	213	MET	2.1
1	C	306	THR	2.1
1	B	217	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	238	ALA	2.1
1	C	81	PRO	2.1
1	C	327	THR	2.1
1	D	349	ALA	2.1
1	B	207	SER	2.1
1	B	533	ASP	2.1
1	A	417	ALA	2.1
1	A	541	GLN	2.1
1	D	415	THR	2.1
1	B	410	PHE	2.1
1	C	410	PHE	2.1
1	B	226	GLY	2.1
1	A	93	ILE	2.0
1	A	370	LEU	2.0
1	D	7	ILE	2.0
1	A	148	ALA	2.0
1	D	167	THR	2.0
1	B	566	LYS	2.0
1	B	210	GLU	2.0
1	A	535	ASP	2.0
1	C	11	SER	2.0
1	A	98	GLY	2.0
1	B	400	GLY	2.0
1	B	569	GLY	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 carbohydrates 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.