Full wwPDB X-ray Structure Validation Report (i)

Oct 27, 2016 – 04:49 PM EDT

|		
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)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
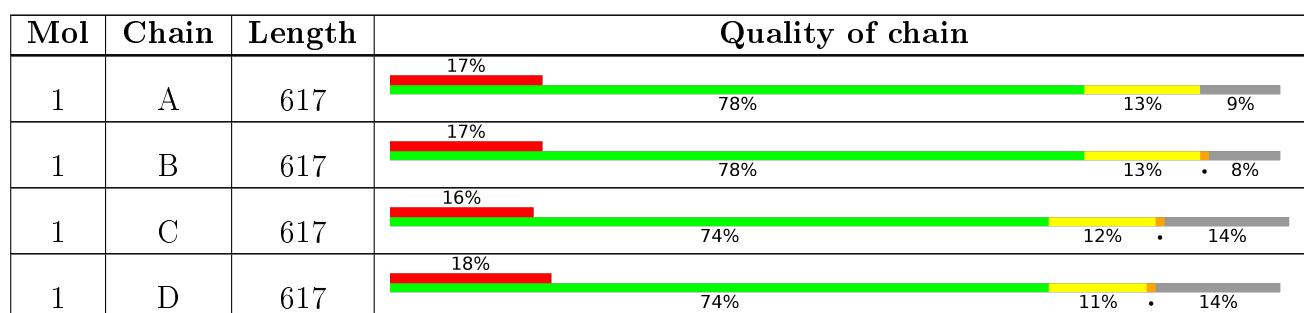
The reported resolution of this entry is 2.00 Å.

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	Percentile Ranks	Value
Rfree		0.243
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		1.9%
RSRZ outliers		19.1%

Worse　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 <=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	17% / 78% 13% 9%
1	B	617	17% / 78% 13% • 8%
1	C	617	16% / 74% 12% • 14%
1	D	617	18% / 74% 11% • 14%

2 Entry composition (i)

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 4419	C 2811	N 738	O 845	S 25	0	0	0
1	B	568	Total 4461	C 2837	N 746	O 852	S 26	0	0	0
1	C	533	Total 4185	C 2663	N 703	O 798	S 21	0	0	0
1	D	532	Total 4174	C 2657	N 700	O 796	S 21	0	0	0

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
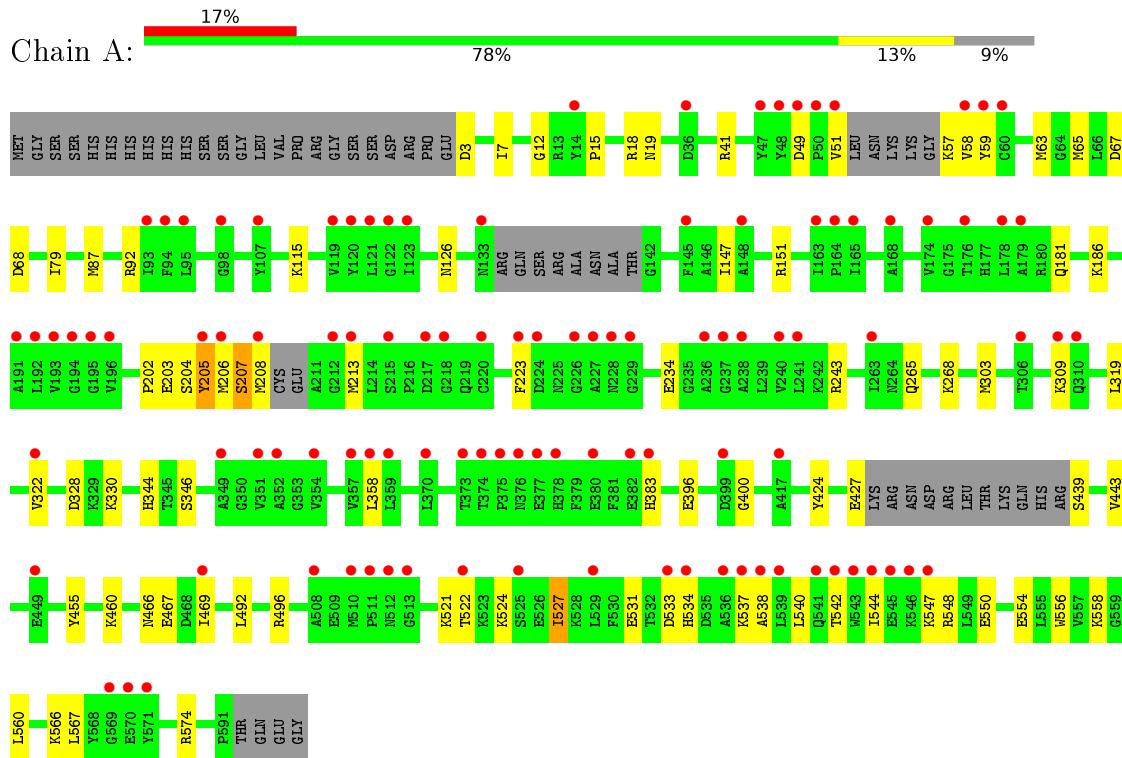
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	371	Total O 371 371	0	0
2	B	333	Total O 333 333	0	0
2	C	320	Total O 320 320	0	0
2	D	334	Total O 334 334	0	0
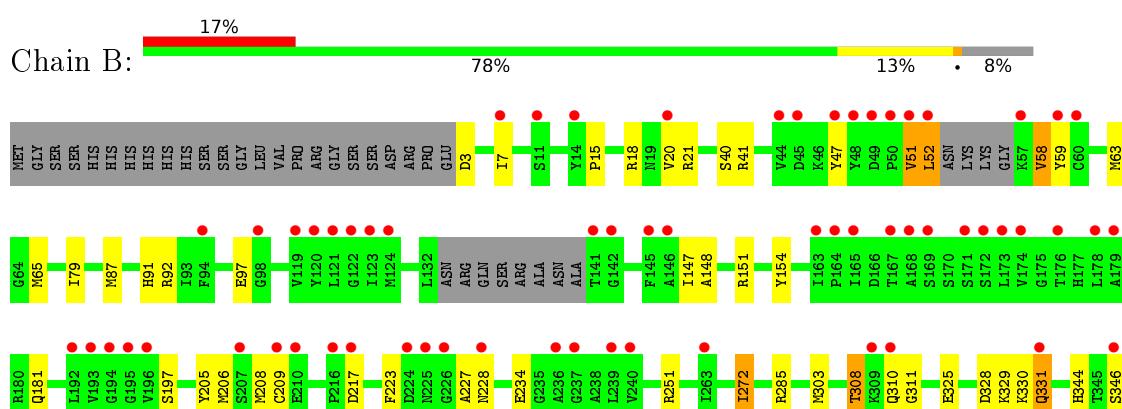
3 Residue-property plots ⓘ
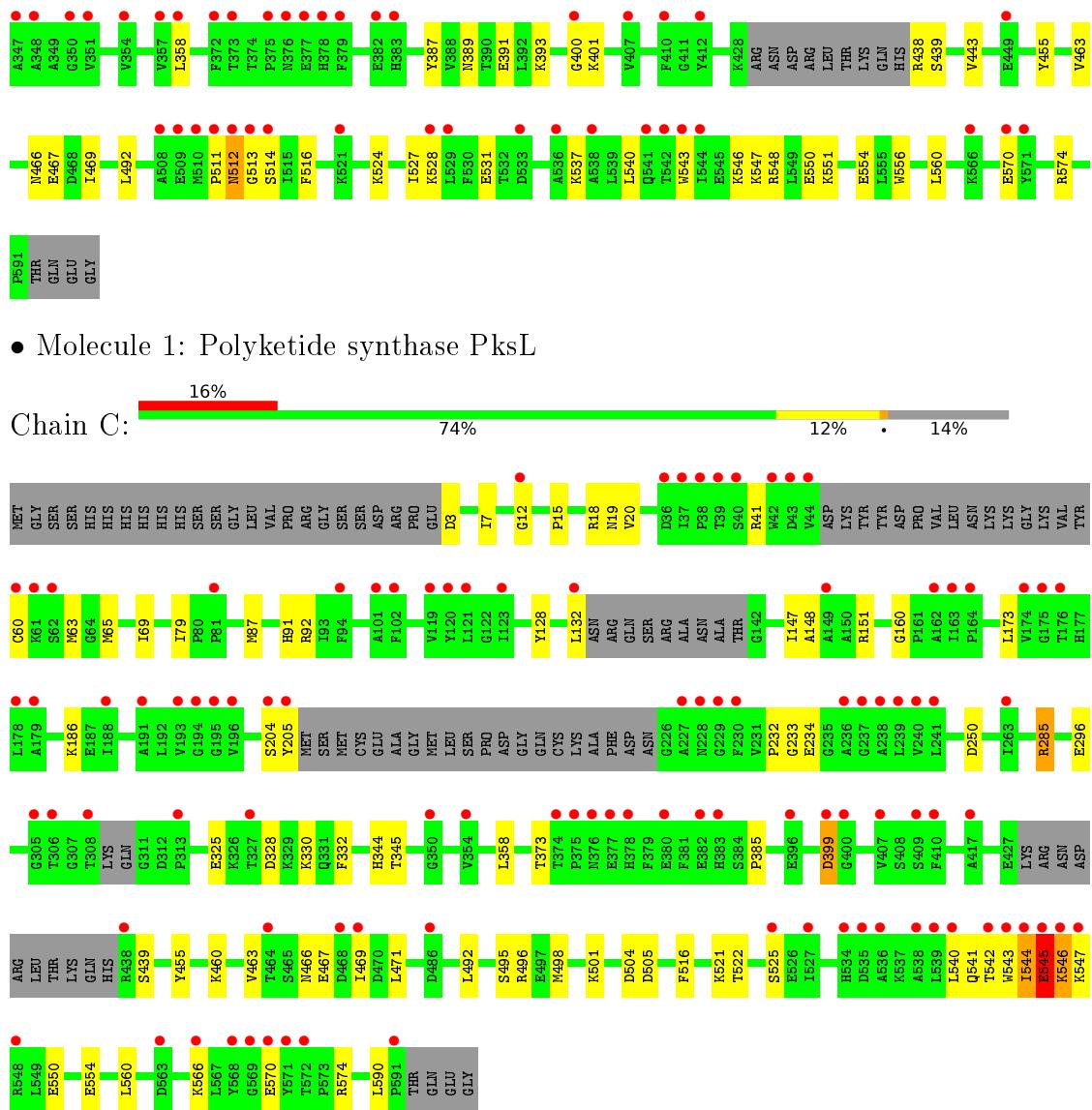
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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
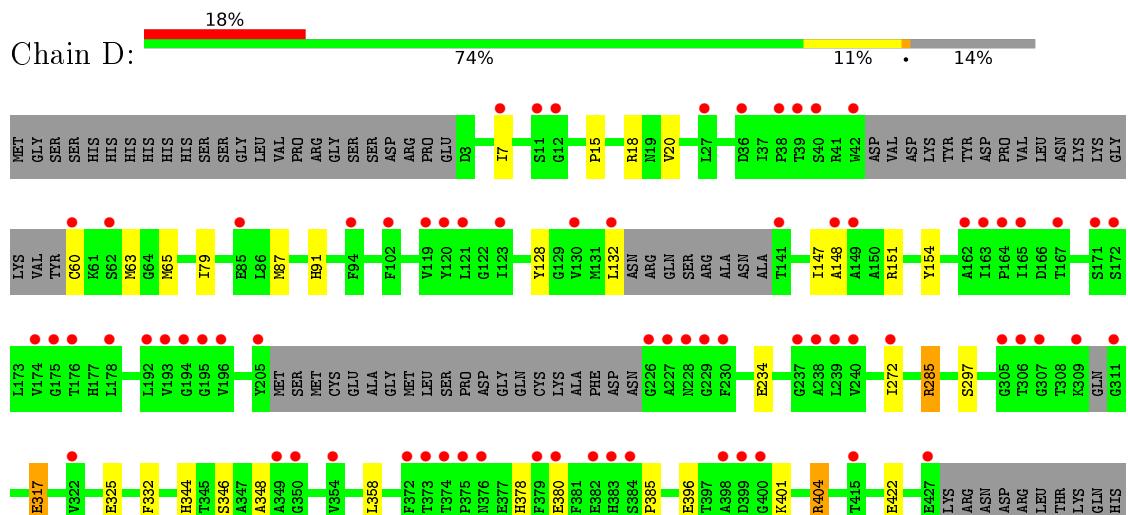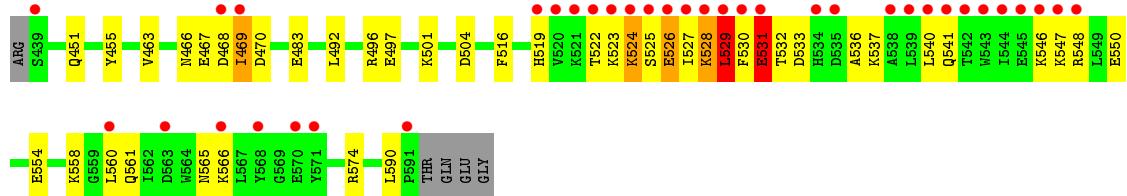
- Molecule 1: Polyketide synthase PksL

• Molecule 1: Polyketide synthase PksL

Chain C:

• Molecule 1: Polyketide synthase PksL

Chain D:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	9700 reflections (5.30%)	DCC
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 , 52.3	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	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.*

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[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 (i)

5.1 Standard geometry (i)

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 (i)

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:546:LYS:O	1:B:546:LYS:CD	2.48	0.61
1:B:543:TRP:CE2	1:B:551:LYS:HD2	2.35	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:533:ASP:O	1:D:537:LYS:CG	2.58	0.48
1:D:529:LEU:HD12	1:D:536:ALA:CB	2.44	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 (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	553/617 (90%)	539 (98%)	13 (2%)	1 (0%)	52	48
1	B	560/617 (91%)	545 (97%)	15 (3%)	0	100	100
1	C	521/617 (84%)	510 (98%)	10 (2%)	1 (0%)	52	48
1	D	520/617 (84%)	504 (97%)	16 (3%)	0	100	100
All	All	2154/2468 (87%)	2098 (97%)	54 (2%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

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

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	468/515 (91%)	463 (99%)	5 (1%)	80	83
1	B	473/515 (92%)	465 (98%)	8 (2%)	68	71
1	C	442/515 (86%)	434 (98%)	8 (2%)	66	69
1	D	441/515 (86%)	428 (97%)	13 (3%)	50	49
All	All	1824/2060 (88%)	1790 (98%)	34 (2%)	65	67

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	563/617 (91%)	0.90	107 (19%)	2	2	23, 37, 68, 106	0
1	B	568/617 (92%)	0.89	104 (18%)	2	2	25, 39, 71, 109	0
1	C	533/617 (86%)	0.90	99 (18%)	2	2	24, 40, 76, 108	0
1	D	532/617 (86%)	1.02	110 (20%)	1	1	25, 39, 71, 106	0
All	All	2196/2468 (88%)	0.93	420 (19%)	2	2	23, 39, 73, 109	0

All (420) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	527	ILE	12.4
1	B	511	PRO	9.3
1	D	535	ASP	8.0
1	D	571	TYR	8.0
1	A	374	THR	7.6
1	C	44	VAL	7.4
1	C	400	GLY	7.3
1	B	512	ASN	7.2
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	6.3
1	C	534	HIS	6.2
1	D	163	ILE	6.1
1	D	529	LEU	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	5.7
1	A	538	ALA	5.6
1	C	374	THR	5.5
1	A	510	MET	5.4
1	A	547	LYS	5.4
1	C	40	SER	5.3
1	D	205	TYR	5.3
1	D	42	TRP	5.3
1	C	132	LEU	5.3
1	D	523	LYS	5.3
1	A	534	HIS	5.2
1	A	544	ILE	5.2
1	D	524	LYS	5.2
1	D	519	HIS	5.1
1	B	50	PRO	5.1
1	B	510	MET	5.1
1	A	373	THR	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	D	373	THR	4.9
1	C	544	ILE	4.9
1	D	374	THR	4.9
1	C	174	VAL	4.9
1	D	531	GLU	4.9
1	D	375	PRO	4.9
1	A	48	TYR	4.9
1	A	163	ILE	4.9
1	C	375	PRO	4.8
1	C	538	ALA	4.8
1	B	174	VAL	4.8
1	B	178	LEU	4.8
1	C	438	ARG	4.8
1	A	60	CYS	4.8
1	A	47	TYR	4.7
1	D	272	ILE	4.7
1	D	39	THR	4.7
1	A	174	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	163	ILE	4.6
1	D	526	GLU	4.6
1	D	538	ALA	4.6
1	D	60	CYS	4.6
1	C	571	TYR	4.6
1	A	217	ASP	4.5
1	B	509	GLU	4.5
1	A	226	GLY	4.5
1	C	542	THR	4.5
1	D	238	ALA	4.5
1	D	547	LYS	4.4
1	A	193	VAL	4.4
1	B	165	ILE	4.4
1	B	48	TYR	4.4
1	A	380	GLU	4.4
1	D	528	LYS	4.3
1	B	351	VAL	4.3
1	A	59	TYR	4.3
1	D	398	ALA	4.3
1	B	173	LEU	4.2
1	D	544	ILE	4.2
1	C	42	TRP	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	C	547	LYS	4.1
1	B	44	VAL	4.1
1	B	163	ILE	4.1
1	B	536	ALA	4.1
1	C	205	TYR	4.1
1	D	520	VAL	4.0
1	A	571	TYR	4.0
1	B	310	GLN	4.0
1	B	528	LYS	3.9
1	D	123	ILE	3.9
1	B	521	LYS	3.9
1	C	238	ALA	3.9
1	B	375	PRO	3.9
1	D	132	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	193	VAL	3.9
1	A	229	GLY	3.9
1	D	38	PRO	3.9
1	A	215	SER	3.9
1	D	176	THR	3.9
1	B	192	LEU	3.9
1	A	569	GLY	3.9
1	C	228	ASN	3.9
1	D	119	VAL	3.9
1	D	307	GLY	3.9
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	C	229	GLY	3.8
1	B	383	HIS	3.7
1	A	513	GLY	3.7
1	D	194	GLY	3.7
1	B	168	ALA	3.7
1	B	377	GLU	3.7
1	D	141	THR	3.7
1	A	196	VAL	3.7
1	C	196	VAL	3.7
1	B	119	VAL	3.7
1	B	239	LEU	3.6
1	B	228	ASN	3.6
1	B	122	GLY	3.6
1	B	195	GLY	3.6
1	B	544	ILE	3.6
1	D	566	LYS	3.6
1	A	205	TYR	3.6
1	D	591	PRO	3.6
1	B	121	LEU	3.6
1	D	534	HIS	3.6
1	C	399	ASP	3.6
1	A	376	ASN	3.5
1	C	60	CYS	3.5
1	A	50	PRO	3.5
1	A	570	GLU	3.5
1	D	469	ILE	3.5

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Full wwPDB X-ray Structure Validation Report

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

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Mol	Chain	Res	Type	RSRZ
1	D	560	LEU	3.2
1	D	548	ARG	3.2
1	A	241	LEU	3.2
1	C	548	ARG	3.2
1	B	449	GLU	3.1
1	C	380	GLU	3.1
1	B	376	ASN	3.1
1	B	94	PHE	3.1
1	D	239	LEU	3.1
1	A	168	ALA	3.1
1	D	149	ALA	3.1
1	A	224	ASP	3.1
1	D	521	LYS	3.1
1	D	382	GLU	3.1
1	A	107	TYR	3.1
1	D	196	VAL	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	A	352	ALA	3.1
1	D	148	ALA	3.1
1	D	383	HIS	3.1
1	C	396	GLU	3.1
1	B	14	TYR	3.1
1	A	191	ALA	3.0
1	A	195	GLY	3.0
1	A	227	ALA	3.0
1	A	176	THR	3.0
1	C	176	THR	3.0
1	A	119	VAL	3.0
1	C	539	LEU	3.0
1	A	51	VAL	3.0
1	C	469	ILE	3.0
1	B	47	TYR	3.0
1	B	120	TYR	3.0
1	C	120	TYR	3.0
1	A	542	THR	3.0
1	C	377	GLU	3.0
1	C	178	LEU	3.0
1	D	193	VAL	3.0
1	D	230	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	354	VAL	3.0
1	D	427	GLU	3.0
1	B	57	LYS	3.0
1	A	164	PRO	2.9
1	D	121	LEU	2.9
1	D	192	LEU	2.9
1	B	209	CYS	2.9
1	C	164	PRO	2.9
1	C	543	TRP	2.9
1	D	162	ALA	2.9
1	C	464	THR	2.9
1	C	204	SER	2.9
1	C	308	THR	2.9
1	B	169	SER	2.9
1	B	357	VAL	2.8
1	C	566	LYS	2.8
1	B	145	PHE	2.8
1	B	542	THR	2.8
1	D	306	THR	2.8
1	A	120	TYR	2.8
1	A	508	ALA	2.8
1	B	172	SER	2.8
1	C	417	ALA	2.8
1	C	149	ALA	2.7
1	D	36	ASP	2.7
1	B	49	ASP	2.7
1	B	538	ALA	2.7
1	D	311	GLY	2.7
1	B	236	ALA	2.7
1	B	379	PHE	2.7
1	D	541	GLN	2.7
1	C	191	ALA	2.7
1	B	60	CYS	2.7
1	C	241	LEU	2.7
1	C	240	VAL	2.7
1	A	145	PHE	2.7
1	D	305	GLY	2.7
1	A	546	LYS	2.7
1	A	539	LEU	2.7
1	D	309	LYS	2.7
1	C	376	ASN	2.7
1	D	570	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	61	LYS	2.6
1	A	529	LEU	2.6
1	B	7	ILE	2.6
1	A	263	ILE	2.6
1	A	469	ILE	2.6
1	C	162	ALA	2.6
1	C	525	SER	2.6
1	B	146	ALA	2.6
1	C	123	ILE	2.6
1	D	226	GLY	2.6
1	A	36	ASP	2.6
1	B	348	ALA	2.6
1	D	178	LEU	2.6
1	B	309	LYS	2.5
1	A	322	VAL	2.5
1	C	119	VAL	2.5
1	A	512	ASN	2.5
1	B	346	SER	2.5
1	C	193	VAL	2.5
1	A	382	GLU	2.5
1	D	563	ASP	2.5
1	C	62	SER	2.5
1	C	350	GLY	2.5
1	C	354	VAL	2.5
1	B	171	SER	2.5
1	C	409	SER	2.5
1	C	179	ALA	2.5
1	A	220	CYS	2.5
1	C	230	PHE	2.5
1	A	236	ALA	2.5
1	B	164	PRO	2.5
1	D	376	ASN	2.5
1	D	439	SER	2.5
1	C	568	TYR	2.5
1	C	175	GLY	2.5
1	A	223	PHE	2.5
1	A	206	MET	2.4
1	A	351	VAL	2.4
1	D	172	SER	2.4
1	C	236	ALA	2.4
1	C	536	ALA	2.4
1	D	227	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	94	PHE	2.4
1	B	240	VAL	2.4
1	A	165	ILE	2.4
1	A	533	ASP	2.4
1	D	372	PHE	2.4
1	B	124	MET	2.4
1	B	358	LEU	2.4
1	C	194	GLY	2.4
1	C	313	PRO	2.4
1	C	37	ILE	2.4
1	A	358	LEU	2.4
1	B	167	THR	2.4
1	D	171	SER	2.4
1	C	94	PHE	2.3
1	A	545	GLU	2.3
1	A	349	ALA	2.3
1	D	568	TYR	2.3
1	B	331	GLN	2.3
1	B	372	PHE	2.3
1	C	239	LEU	2.3
1	C	227	ALA	2.3
1	B	216	PRO	2.3
1	B	11	SER	2.3
1	A	357	VAL	2.3
1	B	20	VAL	2.3
1	C	305	GLY	2.3
1	C	38	PRO	2.3
1	B	142	GLY	2.3
1	D	379	PHE	2.3
1	D	228	ASN	2.3
1	A	58	VAL	2.3
1	A	354	VAL	2.3
1	B	179	ALA	2.3
1	C	382	GLU	2.3
1	D	62	SER	2.3
1	B	225	ASN	2.3
1	A	359	LEU	2.3
1	C	101	ALA	2.3
1	A	522	THR	2.3
1	B	141	THR	2.3
1	D	542	THR	2.3
1	A	543	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	237	GLY	2.3
1	C	263	ILE	2.3
1	A	179	ALA	2.2
1	B	176	THR	2.2
1	B	407	VAL	2.2
1	A	212	GLY	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	D	468	ASP	2.2
1	A	377	GLU	2.2
1	B	224	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	A	122	GLY	2.2
1	A	399	ASP	2.2
1	B	45	ASP	2.2
1	D	11	SER	2.2
1	D	102	PHE	2.2
1	D	240	VAL	2.2
1	A	306	THR	2.2
1	B	347	ALA	2.2
1	D	27	LEU	2.1
1	D	130	VAL	2.1
1	C	36	ASP	2.1
1	B	541	GLN	2.1
1	C	188	ILE	2.1
1	B	217	ASP	2.1
1	D	120	TYR	2.1
1	A	213	MET	2.1
1	D	175	GLY	2.1
1	D	384	SER	2.1
1	D	85	GLU	2.1
1	C	486	ASP	2.1
1	C	306	THR	2.1
1	D	322	VAL	2.1

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