



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:22 AM UTC

PDB ID : 1EK9 / pdb_00001ek9
Title : 2.1A X-RAY STRUCTURE OF TOLC: AN INTEGRAL OUTER MEMBRANE PROTEIN AND EFFLUX PUMP COMPONENT FROM ESCHERICHIA COLI
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Deposited on : 2000-03-07
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

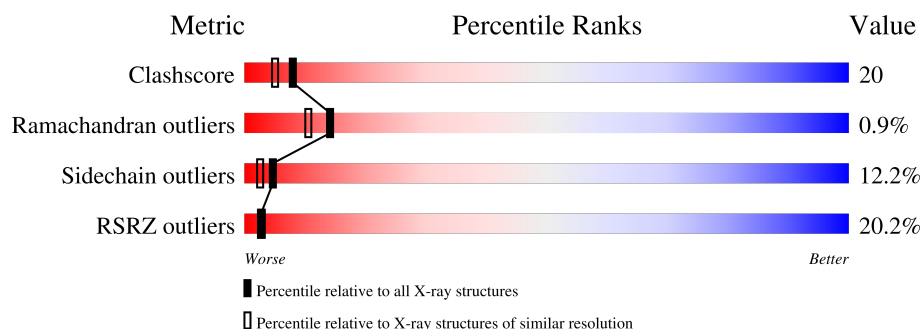
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	428	
1	B	428	
1	C	428	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11426 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 OUTER MEMBRANE PROTEIN TOLC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	Se	0	0	0
			3306	2038	586	677	5			
1	B	428	Total	C	N	O	Se	0	0	0
			3306	2038	586	677	5			
1	C	428	Total	C	N	O	Se	0	0	0
			3306	2038	586	677	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MSE	MET	modified residue	UNP P02930
A	78	MSE	MET	modified residue	UNP P02930
A	279	MSE	MET	modified residue	UNP P02930
A	297	MSE	MET	modified residue	UNP P02930
A	358	MSE	MET	modified residue	UNP P02930
B	4	MSE	MET	modified residue	UNP P02930
B	78	MSE	MET	modified residue	UNP P02930
B	279	MSE	MET	modified residue	UNP P02930
B	297	MSE	MET	modified residue	UNP P02930
B	358	MSE	MET	modified residue	UNP P02930
C	4	MSE	MET	modified residue	UNP P02930
C	78	MSE	MET	modified residue	UNP P02930
C	279	MSE	MET	modified residue	UNP P02930
C	297	MSE	MET	modified residue	UNP P02930
C	358	MSE	MET	modified residue	UNP P02930

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	442	Total	O	0	0
			442	442		
2	B	558	Total	O	0	0
			558	558		

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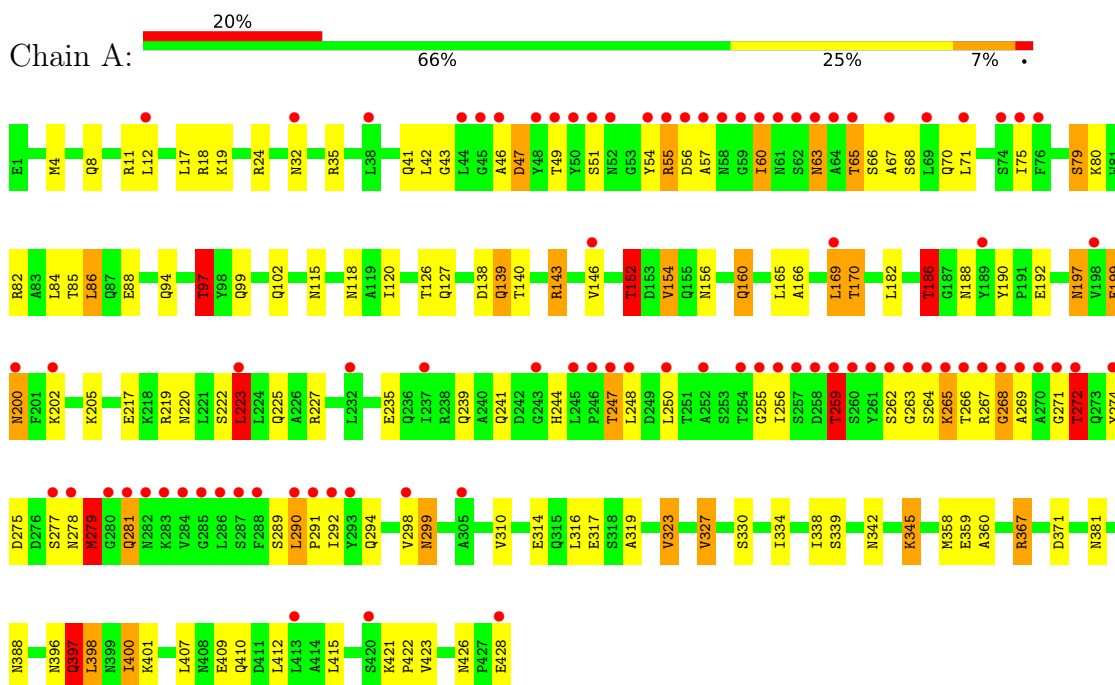
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	508	Total	O	0	0
			508	508		

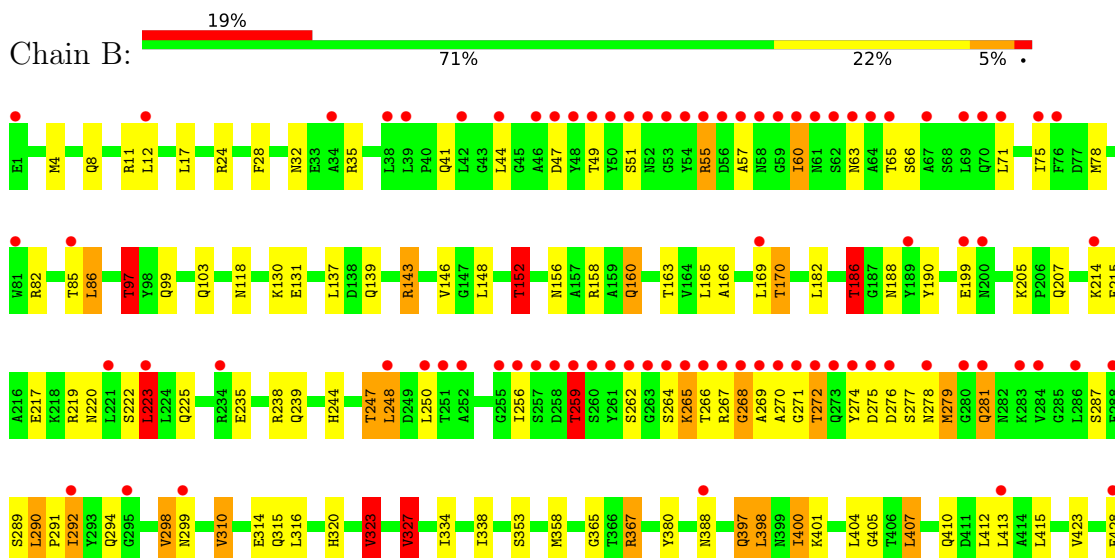
3 Residue-property plots [i](#)

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.

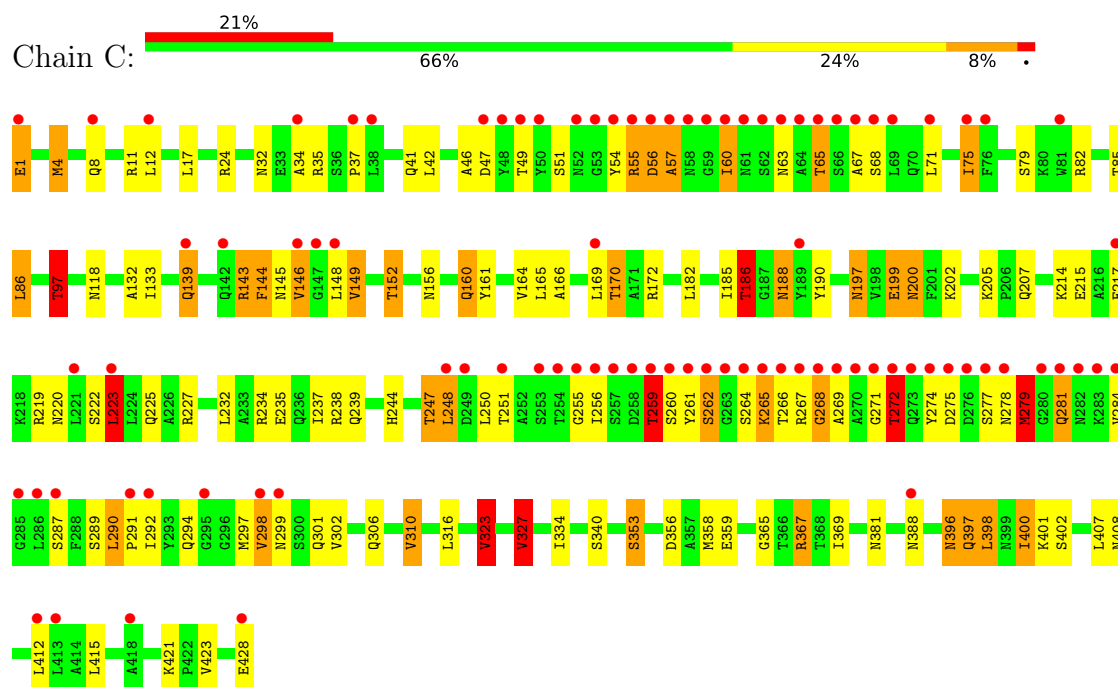
• Molecule 1: OUTER MEMBRANE PROTEIN TOLC



• Molecule 1: OUTER MEMBRANE PROTEIN TOLC



● Molecule 1: OUTER MEMBRANE PROTEIN TOLC



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	265.05Å 265.05Å 95.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.10) 99.5 (20.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.10Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.208 , 0.257 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11426	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	1.15	4/3342 (0.1%)	1.51	22/4530 (0.5%)
1	B	1.15	1/3342 (0.0%)	1.49	22/4530 (0.5%)
1	C	1.17	3/3342 (0.1%)	1.53	36/4530 (0.8%)
All	All	1.16	8/10026 (0.1%)	1.51	80/13590 (0.6%)

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	C	0	5
All	All	0	7

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	GLY	CA-C	6.15	1.57	1.52
1	C	356	ASP	C-O	-5.94	1.17	1.24
1	B	367	ARG	NE-CZ	-5.68	1.26	1.33
1	C	149	VAL	N-CA	5.63	1.52	1.46
1	A	154	VAL	N-CA	5.51	1.53	1.46
1	A	345	LYS	C-O	-5.22	1.18	1.24
1	C	132	ALA	CA-CB	5.14	1.61	1.53
1	A	299	ASN	C-O	-5.08	1.17	1.24

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	367	ARG	NE-CZ-NH1	-11.72	109.78	121.50
1	A	367	ARG	NE-CZ-NH2	10.79	128.91	119.20
1	A	367	ARG	NE-CZ-NH1	-10.72	110.78	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ARG	NE-CZ-NH1	-8.58	112.92	121.50
1	A	259	THR	N-CA-CB	8.29	124.49	110.49
1	A	186	THR	N-CA-CB	-8.04	98.27	110.33
1	C	186	THR	N-CA-CB	-8.00	98.79	110.47
1	B	259	THR	N-CA-CB	7.88	123.81	110.49
1	B	186	THR	N-CA-CB	-7.68	98.81	110.33
1	B	367	ARG	NE-CZ-NH2	7.61	126.05	119.20
1	B	143	ARG	NE-CZ-NH1	7.42	128.92	121.50
1	C	259	THR	N-CA-CB	7.28	122.79	110.49
1	C	327	VAL	N-CA-CB	7.26	121.47	110.58
1	B	428	GLU	N-CA-CB	7.16	122.68	110.50
1	A	428	GLU	N-CA-CB	6.82	122.10	110.50
1	B	99	GLN	CA-C-N	6.53	129.03	120.28
1	B	99	GLN	C-N-CA	6.53	129.03	120.28
1	C	143	ARG	CD-NE-CZ	6.52	133.53	124.40
1	C	149	VAL	N-CA-CB	-6.40	99.46	111.62
1	B	223	LEU	CB-CA-C	6.38	123.40	110.38
1	A	279	MSE	CA-CB-CG	6.35	126.79	114.10
1	C	340	SER	N-CA-CB	6.32	119.18	110.01
1	A	115	ASN	N-CA-CB	6.24	119.95	110.28
1	C	428	GLU	N-CA-CB	6.22	121.08	110.50
1	B	323	VAL	N-CA-CB	6.18	120.89	110.56
1	A	143	ARG	NE-CZ-NH2	-6.16	113.66	119.20
1	A	97	THR	N-CA-CB	6.14	119.68	110.22
1	B	152	THR	CA-CB-OG1	6.09	118.73	109.60
1	C	56	ASP	CA-CB-CG	6.09	118.69	112.60
1	C	97	THR	N-CA-CB	6.06	119.67	110.28
1	C	144	PHE	O-C-N	-6.06	115.73	122.03
1	B	327	VAL	N-CA-CB	5.97	119.53	110.58
1	A	143	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	C	188	ASN	N-CA-C	5.93	119.22	109.85
1	C	284	VAL	N-CA-CB	5.93	121.01	111.23
1	A	397	GLN	CB-CA-C	-5.92	100.79	110.85
1	C	272	THR	CA-C-N	5.76	128.79	120.38
1	C	272	THR	C-N-CA	5.76	128.79	120.38
1	A	360	ALA	N-CA-C	-5.75	105.09	111.36
1	C	323	VAL	N-CA-CB	5.73	121.78	110.95
1	A	272	THR	CA-C-N	5.70	128.19	120.38
1	A	272	THR	C-N-CA	5.70	128.19	120.38
1	C	143	ARG	N-CA-C	-5.67	105.25	111.82
1	A	152	THR	N-CA-C	5.65	118.17	111.33
1	C	57	ALA	N-CA-C	-5.62	105.34	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	ILE	N-CA-C	-5.60	106.75	111.56
1	C	237	ILE	N-CA-C	-5.56	105.30	110.53
1	C	421	LYS	N-CA-C	5.56	117.75	110.08
1	C	298	VAL	CA-C-O	-5.55	113.84	120.78
1	B	97	THR	N-CA-CB	5.47	118.17	110.12
1	C	367	ARG	NH1-CZ-NH2	5.44	126.37	119.30
1	C	143	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	B	152	THR	OG1-CB-CG2	5.35	119.99	109.30
1	C	223	LEU	CB-CA-C	5.33	121.14	109.99
1	A	56	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	143	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	B	405	GLY	N-CA-C	-5.25	107.98	115.64
1	A	143	ARG	CD-NE-CZ	5.24	131.74	124.40
1	A	223	LEU	CB-CA-C	5.24	121.07	110.38
1	C	1	GLU	CA-C-O	-5.22	111.92	120.80
1	C	185	ILE	CA-C-O	5.22	126.29	120.71
1	C	145	ASN	CA-CB-CG	-5.21	107.39	112.60
1	A	152	THR	OG1-CB-CG2	5.19	119.68	109.30
1	A	126	THR	N-CA-C	-5.19	105.70	111.36
1	B	78	MSE	CG-SE-CE	-5.18	87.53	98.92
1	C	369	ILE	N-CA-C	-5.18	104.62	111.09
1	C	367	ARG	CD-NE-CZ	5.18	131.65	124.40
1	A	63	ASN	CB-CA-C	5.16	118.09	110.14
1	C	367	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	C	310	VAL	CA-C-N	5.16	125.81	120.03
1	C	310	VAL	C-N-CA	5.16	125.81	120.03
1	B	310	VAL	CA-C-N	5.14	125.68	119.98
1	B	310	VAL	C-N-CA	5.14	125.68	119.98
1	C	396	ASN	CA-CB-CG	-5.10	107.50	112.60
1	B	380	TYR	CA-CB-CG	-5.07	104.78	113.90
1	B	292	ILE	CA-C-O	-5.05	114.47	120.78
1	B	298	VAL	O-C-N	-5.05	116.26	122.57
1	B	310	VAL	N-CA-CB	5.05	118.15	110.58
1	C	145	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	152	THR	CA-CB-OG1	5.03	117.14	109.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	314	GLU	Mainchain
1	A	317	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	C	144	PHE	Mainchain
1	C	34	ALA	Mainchain
1	C	353	SER	Mainchain
1	C	402	SER	Mainchain
1	C	97	THR	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	3306	0	3256	141	0
1	B	3306	0	3256	132	0
1	C	3306	0	3256	147	0
2	A	442	0	0	41	2
2	B	558	0	0	45	1
2	C	508	0	0	54	1
All	All	11426	0	9768	385	2

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 20.

All (385) 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:B:156:ASN:HD21	1:C:367:ARG:NH1	1.34	1.23
1:B:423:VAL:HB	2:B:703:HOH:O	1.40	1.19
1:A:156:ASN:HD21	1:B:367:ARG:NH1	1.42	1.17
1:C:423:VAL:HB	2:C:624:HOH:O	1.42	1.16
1:A:367:ARG:NH1	1:C:156:ASN:HD21	1.46	1.14
1:B:146:VAL:HB	2:B:952:HOH:O	1.47	1.12
1:B:265:LYS:HG2	2:B:971:HOH:O	1.49	1.10
1:A:146:VAL:HB	2:A:750:HOH:O	1.55	1.03
1:C:388:ASN:HB2	2:C:525:HOH:O	1.61	0.99
1:A:426:ASN:HB2	2:A:803:HOH:O	1.65	0.97
1:B:156:ASN:ND2	1:C:367:ARG:NH1	2.11	0.96
1:B:156:ASN:HD21	1:C:367:ARG:HH12	1.05	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:THR:HG22	1:B:225:GLN:NE2	1.82	0.93
1:B:118:ASN:HD21	1:B:388:ASN:HD22	1.18	0.91
1:C:79:SER:HA	2:C:933:HOH:O	1.70	0.91
1:B:388:ASN:HB2	2:B:520:HOH:O	1.69	0.90
1:C:57:ALA:HB3	2:C:695:HOH:O	1.70	0.89
1:B:156:ASN:ND2	1:C:367:ARG:HH12	1.70	0.89
1:A:156:ASN:ND2	1:B:367:ARG:NH1	2.22	0.88
1:A:415:LEU:HD21	2:A:609:HOH:O	1.75	0.87
1:C:118:ASN:HD21	1:C:388:ASN:HD22	1.23	0.87
1:A:298:VAL:O	1:A:299:ASN:HB2	1.75	0.86
1:B:85:THR:HG22	2:B:581:HOH:O	1.75	0.86
1:A:118:ASN:HD21	1:A:388:ASN:HD22	1.22	0.85
1:A:156:ASN:HD21	1:B:367:ARG:HH12	1.20	0.84
1:A:227:ARG:HD3	2:A:721:HOH:O	1.75	0.84
1:A:421:LYS:HE3	2:A:787:HOH:O	1.78	0.84
1:A:97:THR:HG22	1:A:225:GLN:NE2	1.94	0.82
1:A:367:ARG:NH1	1:C:156:ASN:ND2	2.27	0.81
1:A:381:ASN:HB3	2:A:500:HOH:O	1.80	0.81
1:C:97:THR:HG22	1:C:225:GLN:NE2	1.96	0.81
1:C:160:GLN:HG3	2:C:875:HOH:O	1.81	0.81
1:A:186:THR:HG22	1:A:188:ASN:H	1.45	0.80
1:B:160:GLN:HG3	2:B:596:HOH:O	1.83	0.79
1:C:139:GLN:NE2	1:C:143:ARG:NH2	2.33	0.77
1:C:388:ASN:HB2	2:C:504:HOH:O	1.82	0.77
1:B:186:THR:HG22	1:B:188:ASN:H	1.48	0.77
1:B:130:LYS:CE	2:B:937:HOH:O	2.32	0.77
1:C:398:LEU:HD11	1:C:415:LEU:HD11	1.66	0.77
1:A:334:ILE:HD12	1:A:400:ILE:HD12	1.66	0.76
1:A:85:THR:HG22	2:A:736:HOH:O	1.85	0.76
1:B:97:THR:HG22	1:B:225:GLN:HE22	1.49	0.76
1:A:160:GLN:HG3	2:A:784:HOH:O	1.84	0.76
1:B:130:LYS:HE2	2:B:937:HOH:O	1.85	0.75
1:C:186:THR:HG22	1:C:188:ASN:H	1.52	0.75
1:C:139:GLN:NE2	1:C:143:ARG:HH22	1.84	0.74
1:B:367:ARG:NE	2:B:934:HOH:O	2.21	0.74
1:C:139:GLN:HE21	1:C:143:ARG:NH2	1.86	0.74
1:C:267:ARG:NE	2:C:925:HOH:O	2.20	0.74
1:A:127:GLN:NE2	2:A:832:HOH:O	2.21	0.74
1:B:139:GLN:NE2	1:B:143:ARG:NH2	2.35	0.74
1:C:85:THR:HG22	2:C:533:HOH:O	1.87	0.74
1:C:186:THR:HG21	1:C:190:TYR:HE1	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLN:NE2	1:A:143:ARG:NH2	2.36	0.73
1:A:165:LEU:O	1:A:169:LEU:HD22	1.89	0.73
1:B:298:VAL:O	1:B:299:ASN:HB2	1.88	0.73
1:A:358:MSE:SE	1:A:367:ARG:HD2	2.39	0.73
1:B:244:HIS:HE1	2:B:621:HOH:O	1.72	0.73
1:C:65:THR:HG21	2:C:921:HOH:O	1.89	0.72
1:B:367:ARG:NH2	2:B:934:HOH:O	2.22	0.72
1:C:133:ILE:HD11	2:C:850:HOH:O	1.89	0.72
1:A:65:THR:HG22	2:A:515:HOH:O	1.89	0.72
1:B:367:ARG:CZ	2:B:934:HOH:O	2.36	0.72
1:A:398:LEU:HD11	1:A:415:LEU:HD11	1.71	0.71
1:B:118:ASN:HD21	1:B:388:ASN:ND2	1.87	0.71
1:A:4:MSE:HG3	2:A:700:HOH:O	1.89	0.70
1:B:220:ASN:HD21	1:B:222:SER:HB2	1.56	0.70
1:C:298:VAL:O	1:C:299:ASN:HB2	1.91	0.70
1:C:220:ASN:HD22	1:C:223:LEU:H	1.40	0.70
1:B:410:GLN:HG2	2:B:627:HOH:O	1.91	0.70
1:C:146:VAL:CG2	2:C:629:HOH:O	2.39	0.70
1:C:146:VAL:HG23	2:C:629:HOH:O	1.92	0.69
1:B:169:LEU:HD13	2:B:648:HOH:O	1.93	0.68
1:C:398:LEU:CD1	1:C:415:LEU:HD11	2.23	0.68
1:A:219:ARG:HD2	2:A:571:HOH:O	1.94	0.68
1:A:220:ASN:HD22	1:A:223:LEU:H	1.38	0.68
1:B:413:LEU:CD2	2:B:823:HOH:O	2.41	0.68
1:A:220:ASN:HD21	1:A:222:SER:HB2	1.58	0.68
1:C:220:ASN:HD21	1:C:222:SER:HB2	1.59	0.68
1:A:186:THR:HG21	1:A:190:TYR:HE1	1.59	0.67
1:C:269:ALA:HB1	2:C:888:HOH:O	1.95	0.67
1:C:358:MSE:SE	1:C:367:ARG:HH11	2.28	0.67
1:C:265:LYS:HE3	1:C:265:LYS:HA	1.77	0.67
1:B:220:ASN:HD22	1:B:223:LEU:H	1.43	0.67
1:A:170:THR:HG21	2:B:508:HOH:O	1.94	0.66
1:C:32:ASN:HD22	1:C:35:ARG:HH22	1.41	0.66
1:C:397:GLN:HE21	1:C:397:GLN:HA	1.60	0.66
1:A:244:HIS:HE1	2:A:514:HOH:O	1.76	0.66
1:B:244:HIS:HD2	2:B:836:HOH:O	1.79	0.66
1:C:169:LEU:HD13	2:C:728:HOH:O	1.95	0.66
1:B:32:ASN:HD22	1:B:35:ARG:HH22	1.42	0.65
1:A:156:ASN:HD21	1:B:367:ARG:CZ	2.09	0.65
1:A:156:ASN:ND2	1:B:367:ARG:CZ	2.61	0.64
1:A:367:ARG:CZ	1:C:156:ASN:HD21	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:GLN:HE21	1:B:143:ARG:NH2	1.92	0.64
1:C:267:ARG:HG2	2:C:925:HOH:O	1.97	0.64
1:C:381:ASN:HB3	2:C:585:HOH:O	1.97	0.64
1:B:186:THR:CG2	1:B:188:ASN:H	2.11	0.64
1:B:413:LEU:HD22	2:B:823:HOH:O	1.98	0.64
1:C:281:GLN:HA	1:C:281:GLN:HE21	1.62	0.64
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.78	0.64
1:C:271:GLY:O	1:C:272:THR:HB	1.97	0.63
1:A:41:GLN:HE22	1:B:294:GLN:HB3	1.63	0.63
1:A:398:LEU:CD1	1:A:415:LEU:HD11	2.28	0.63
1:A:367:ARG:NH1	1:C:152:THR:OG1	2.32	0.63
1:B:398:LEU:CD1	1:B:415:LEU:HD11	2.29	0.63
1:C:267:ARG:CG	2:C:925:HOH:O	2.47	0.63
1:A:156:ASN:ND2	1:B:367:ARG:HH12	1.91	0.62
1:A:192:GLU:HB2	2:A:868:HOH:O	1.99	0.62
1:C:182:LEU:O	1:C:186:THR:HB	1.99	0.62
1:A:367:ARG:HH12	1:C:156:ASN:HD21	1.39	0.62
1:B:165:LEU:O	1:B:169:LEU:HD22	1.98	0.62
1:C:1:GLU:N	2:C:463:HOH:O	2.33	0.62
1:A:186:THR:CG2	1:A:188:ASN:H	2.11	0.62
1:A:244:HIS:HD2	2:A:845:HOH:O	1.83	0.61
1:C:172:ARG:HB2	2:C:720:HOH:O	2.01	0.61
1:A:281:GLN:HE21	1:A:281:GLN:HA	1.66	0.61
1:B:186:THR:HG21	1:B:190:TYR:HE1	1.64	0.60
1:B:268:GLY:O	1:B:269:ALA:HB3	2.01	0.60
1:B:281:GLN:HA	1:B:281:GLN:HE21	1.65	0.60
1:C:398:LEU:HD11	1:C:415:LEU:CD1	2.32	0.60
1:C:247:THR:HG23	1:C:289:SER:HB3	1.82	0.59
1:A:97:THR:HG22	1:A:225:GLN:HE22	1.64	0.59
1:A:367:ARG:CZ	1:C:156:ASN:ND2	2.64	0.59
1:A:397:GLN:HA	1:A:397:GLN:HE21	1.67	0.59
1:B:205:LYS:HD2	2:B:655:HOH:O	2.02	0.59
1:C:165:LEU:O	1:C:169:LEU:HD22	2.03	0.59
1:C:186:THR:HG21	1:C:190:TYR:CE1	2.37	0.59
1:A:290:LEU:HD13	1:A:292:ILE:HG13	1.85	0.58
1:A:118:ASN:HD21	1:A:388:ASN:ND2	1.96	0.58
1:A:32:ASN:HD22	1:A:35:ARG:HH22	1.51	0.58
1:B:130:LYS:NZ	2:B:937:HOH:O	2.20	0.58
1:B:57:ALA:O	1:B:60:ILE:HG22	2.04	0.58
1:B:290:LEU:HD13	1:B:292:ILE:HG13	1.85	0.58
1:A:118:ASN:ND2	1:A:388:ASN:HD22	1.99	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:SER:HA	2:A:811:HOH:O	2.04	0.57
1:C:207:GLN:NE2	2:C:927:HOH:O	2.37	0.57
1:B:410:GLN:NE2	2:B:728:HOH:O	2.36	0.57
1:B:320:HIS:HB2	2:B:681:HOH:O	2.04	0.57
1:A:4:MSE:O	1:A:8:GLN:HG2	2.05	0.57
1:B:247:THR:CG2	1:B:289:SER:HB3	2.35	0.57
1:B:244:HIS:O	2:B:966:HOH:O	2.17	0.56
1:C:290:LEU:HD13	1:C:292:ILE:HG13	1.87	0.56
1:A:265:LYS:HG3	2:A:775:HOH:O	2.05	0.56
1:B:397:GLN:HE21	1:B:397:GLN:HA	1.69	0.56
1:C:160:GLN:NE2	2:C:509:HOH:O	2.39	0.56
1:C:4:MSE:O	1:C:8:GLN:HG2	2.06	0.56
1:A:268:GLY:O	1:A:269:ALA:HB3	2.06	0.56
1:C:197:ASN:C	1:C:197:ASN:HD22	2.14	0.56
1:A:342:ASN:ND2	2:A:747:HOH:O	2.38	0.55
1:B:156:ASN:ND2	1:C:367:ARG:CZ	2.69	0.55
1:B:334:ILE:HD12	1:B:400:ILE:HD12	1.87	0.55
1:B:4:MSE:O	1:B:8:GLN:HG2	2.07	0.55
1:C:219:ARG:HD2	2:C:913:HOH:O	2.07	0.55
1:A:182:LEU:C	1:A:182:LEU:HD13	2.32	0.55
1:B:41:GLN:HE22	1:C:294:GLN:HB3	1.71	0.55
1:A:146:VAL:O	1:A:146:VAL:HG22	2.07	0.55
1:A:120:ILE:HG21	1:A:423:VAL:HG11	1.89	0.55
1:B:265:LYS:HE3	1:B:265:LYS:HA	1.88	0.55
1:C:215:GLU:OE1	1:C:219:ARG:NH1	2.40	0.55
1:A:294:GLN:HB3	1:C:41:GLN:HE22	1.71	0.55
1:B:398:LEU:HD13	1:B:415:LEU:HD11	1.88	0.55
1:A:60:ILE:HD12	1:A:274:TYR:CE1	2.42	0.54
1:A:186:THR:HG21	1:A:190:TYR:CE1	2.40	0.54
1:B:170:THR:HG21	2:C:546:HOH:O	2.05	0.54
1:B:247:THR:HG23	1:B:289:SER:HB3	1.88	0.54
1:A:170:THR:CG2	2:B:508:HOH:O	2.55	0.54
1:C:8:GLN:NE2	2:C:908:HOH:O	2.38	0.54
1:C:170:THR:HG21	2:C:466:HOH:O	2.08	0.54
1:C:408:ASN:HB2	2:C:707:HOH:O	2.07	0.54
1:B:265:LYS:HD2	2:B:935:HOH:O	2.07	0.53
1:A:410:GLN:HG2	2:A:847:HOH:O	2.08	0.53
1:B:182:LEU:O	1:B:186:THR:HB	2.09	0.53
1:B:290:LEU:HD22	1:B:291:PRO:HD2	1.90	0.53
1:B:215:GLU:OE1	1:B:219:ARG:NH1	2.42	0.53
1:B:131:GLU:HB3	2:B:571:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:HD11	1:A:415:LEU:CD1	2.39	0.53
1:C:274:TYR:CD2	2:C:896:HOH:O	2.62	0.52
1:A:422:PRO:HB3	2:A:868:HOH:O	2.09	0.52
1:B:250:LEU:HD23	1:B:250:LEU:C	2.35	0.52
1:B:57:ALA:HB2	1:C:279:MSE:HE3	1.91	0.52
1:A:197:ASN:ND2	1:A:200:ASN:H	2.07	0.52
1:C:323:VAL:O	1:C:327:VAL:HG13	2.09	0.52
1:A:290:LEU:HD22	1:A:291:PRO:HD2	1.91	0.51
1:B:44:LEU:HB2	1:C:292:ILE:HD11	1.91	0.51
1:A:279:MSE:CE	2:A:661:HOH:O	2.58	0.51
1:A:247:THR:HG23	1:A:289:SER:HB3	1.92	0.51
1:C:65:THR:HG22	2:C:777:HOH:O	2.10	0.51
1:A:182:LEU:O	1:A:186:THR:HB	2.10	0.51
1:C:244:HIS:HE1	2:C:899:HOH:O	1.93	0.51
1:B:267:ARG:NH2	1:B:275:ASP:HA	2.26	0.51
1:A:334:ILE:HG13	1:A:396:ASN:HB3	1.93	0.51
1:C:234:ARG:NH1	2:C:667:HOH:O	2.32	0.51
1:C:388:ASN:CB	2:C:504:HOH:O	2.50	0.51
1:A:166:ALA:HA	1:A:169:LEU:HD23	1.93	0.50
1:B:207:GLN:HG3	2:B:845:HOH:O	2.11	0.50
1:C:264:SER:OG	1:C:265:LYS:N	2.42	0.50
1:B:398:LEU:HD11	1:B:415:LEU:HD11	1.93	0.50
1:A:205:LYS:HD3	1:A:338:ILE:HD13	1.92	0.50
1:B:139:GLN:NE2	1:B:143:ARG:HH22	2.08	0.50
1:C:49:THR:O	1:C:63:ASN:HA	2.11	0.50
1:B:166:ALA:HA	1:B:169:LEU:HD23	1.94	0.50
1:C:118:ASN:HD21	1:C:388:ASN:ND2	2.00	0.50
1:C:260:SER:HB3	2:C:916:HOH:O	2.12	0.50
1:A:57:ALA:O	1:A:60:ILE:HG22	2.12	0.50
1:B:423:VAL:HG13	2:B:680:HOH:O	2.12	0.50
1:C:234:ARG:NH2	2:C:825:HOH:O	2.43	0.50
1:A:86:LEU:HD13	1:A:235:GLU:HG3	1.94	0.50
1:A:182:LEU:HD13	1:A:182:LEU:O	2.12	0.50
1:B:28:PHE:HD2	2:B:852:HOH:O	1.94	0.50
1:A:139:GLN:NE2	1:A:143:ARG:HH22	2.09	0.49
1:C:186:THR:CG2	1:C:188:ASN:H	2.21	0.49
1:A:49:THR:O	1:A:63:ASN:HA	2.12	0.49
1:A:138:ASP:OD2	2:A:818:HOH:O	2.20	0.49
1:B:276:ASP:HB3	2:B:956:HOH:O	2.12	0.49
1:C:397:GLN:HE21	1:C:397:GLN:CA	2.24	0.49
1:B:223:LEU:CD1	2:B:663:HOH:O	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLU:CD	2:C:574:HOH:O	2.56	0.49
1:A:400:ILE:HG22	2:A:602:HOH:O	2.11	0.49
1:A:247:THR:CG2	1:A:289:SER:HB3	2.42	0.49
1:A:4:MSE:CG	2:A:700:HOH:O	2.55	0.49
1:B:186:THR:HG21	1:B:190:TYR:CE1	2.47	0.48
1:B:358:MSE:SE	1:B:367:ARG:HH11	2.46	0.48
1:A:241:GLN:HG2	2:A:776:HOH:O	2.13	0.48
1:A:82:ARG:HG2	1:A:239:GLN:HB2	1.95	0.48
1:B:82:ARG:HG2	1:B:239:GLN:HB2	1.95	0.48
1:A:223:LEU:HD11	2:A:801:HOH:O	2.14	0.48
2:A:474:HOH:O	1:C:152:THR:HB	2.13	0.48
1:B:55:ARG:O	1:C:278:ASN:O	2.32	0.48
1:B:165:LEU:HD12	2:B:633:HOH:O	2.13	0.48
1:C:37:PRO:HG2	2:C:688:HOH:O	2.12	0.48
1:A:152:THR:HG21	2:B:432:HOH:O	2.13	0.48
1:B:223:LEU:HD12	2:B:663:HOH:O	2.14	0.48
1:A:334:ILE:HD12	1:A:400:ILE:CD1	2.41	0.48
1:A:99:GLN:NE2	2:A:668:HOH:O	2.46	0.48
1:B:388:ASN:HB2	2:B:597:HOH:O	2.12	0.48
1:C:269:ALA:CB	2:C:888:HOH:O	2.58	0.48
1:C:60:ILE:HD12	1:C:274:TYR:CE1	2.48	0.47
1:C:275:ASP:N	2:C:797:HOH:O	2.47	0.47
1:A:223:LEU:CD1	2:A:801:HOH:O	2.61	0.47
1:B:271:GLY:O	1:B:272:THR:HB	2.13	0.47
1:C:247:THR:CG2	1:C:289:SER:HB3	2.43	0.47
1:A:140:THR:HG22	1:A:154:VAL:HG22	1.96	0.47
1:A:323:VAL:O	1:A:327:VAL:HG13	2.15	0.47
1:C:75:ILE:HG21	1:C:248:LEU:HD12	1.97	0.47
1:B:152:THR:HG21	2:C:431:HOH:O	2.14	0.47
1:A:19:LYS:HE3	1:B:315:GLN:NE2	2.29	0.47
1:A:267:ARG:NH2	1:A:275:ASP:HA	2.29	0.47
1:C:79:SER:CB	2:C:933:HOH:O	2.62	0.47
1:C:323:VAL:HG12	2:C:807:HOH:O	2.15	0.47
1:B:223:LEU:HD12	1:B:223:LEU:C	2.40	0.46
1:A:197:ASN:ND2	1:A:199:GLU:HG2	2.31	0.46
1:A:264:SER:OG	1:A:265:LYS:N	2.49	0.46
1:A:250:LEU:C	1:A:250:LEU:HD23	2.41	0.46
1:C:161:TYR:O	1:C:164:VAL:HG12	2.15	0.46
1:C:267:ARG:HB3	1:C:268:GLY:H	1.61	0.46
1:C:8:GLN:OE1	1:C:11:ARG:NH2	2.49	0.46
1:C:397:GLN:HA	1:C:397:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:THR:HG22	1:C:225:GLN:HE22	1.75	0.46
1:A:345:LYS:NZ	2:A:747:HOH:O	2.48	0.46
1:C:261:TYR:O	1:C:262:SER:HB3	2.15	0.46
1:C:334:ILE:HG13	1:C:396:ASN:HB3	1.97	0.46
1:B:235:GLU:OE2	1:B:238:ARG:NH1	2.49	0.46
1:B:49:THR:O	1:B:63:ASN:HA	2.15	0.45
1:A:267:ARG:HB3	1:A:268:GLY:H	1.68	0.45
1:B:146:VAL:HG22	1:B:146:VAL:O	2.16	0.45
1:B:265:LYS:O	1:B:265:LYS:HG3	2.17	0.45
1:A:381:ASN:ND2	2:A:722:HOH:O	2.44	0.45
1:C:199:GLU:H	1:C:199:GLU:HG2	1.50	0.45
1:C:223:LEU:C	1:C:223:LEU:HD12	2.41	0.45
1:C:334:ILE:HD12	1:C:400:ILE:HD12	1.97	0.45
1:A:279:MSE:HE2	2:A:661:HOH:O	2.16	0.45
1:B:265:LYS:CD	2:B:935:HOH:O	2.64	0.45
1:A:94:GLN:NE2	2:A:731:HOH:O	2.50	0.45
1:A:139:GLN:HE21	1:A:143:ARG:NH2	2.13	0.45
1:C:301:GLN:NE2	2:C:730:HOH:O	2.49	0.45
1:A:152:THR:OG1	1:B:367:ARG:NH1	2.50	0.45
1:C:160:GLN:HE21	1:C:160:GLN:HB2	1.35	0.45
1:C:223:LEU:HD13	1:C:227:ARG:NH1	2.32	0.45
1:C:265:LYS:O	1:C:265:LYS:HG3	2.16	0.45
1:C:146:VAL:HG13	1:C:148:LEU:HG	1.99	0.45
1:C:297:MSE:C	1:C:298:VAL:O	2.55	0.44
1:A:102:GLN:HG2	2:A:598:HOH:O	2.17	0.44
1:C:223:LEU:CD1	1:C:227:ARG:NH1	2.80	0.44
1:A:55:ARG:O	1:B:278:ASN:O	2.35	0.44
1:C:182:LEU:O	1:C:182:LEU:HD13	2.17	0.44
1:C:223:LEU:CD1	2:C:873:HOH:O	2.66	0.44
1:A:278:ASN:HB3	1:C:55:ARG:CZ	2.48	0.44
1:A:339:SER:HB3	1:C:169:LEU:CD1	2.47	0.44
1:B:267:ARG:HB3	1:B:268:GLY:H	1.72	0.44
1:C:46:ALA:HA	1:C:67:ALA:HA	2.00	0.44
1:A:265:LYS:HG3	1:A:265:LYS:O	2.18	0.44
1:B:205:LYS:HD3	1:B:338:ILE:HD13	1.99	0.44
1:C:166:ALA:HA	1:C:169:LEU:HD23	1.99	0.44
1:A:24:ARG:HA	1:A:94:GLN:HG3	1.99	0.43
1:B:143:ARG:HA	1:B:146:VAL:HG12	1.99	0.43
1:C:268:GLY:O	1:C:269:ALA:HB3	2.18	0.43
1:C:359:GLU:OE2	2:C:706:HOH:O	2.21	0.43
1:C:290:LEU:HD22	1:C:291:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ARG:NE	2:B:692:HOH:O	2.52	0.43
1:C:182:LEU:HD13	1:C:182:LEU:C	2.44	0.43
1:C:358:MSE:SE	1:C:367:ARG:HD2	2.68	0.43
1:B:24:ARG:HE	1:B:24:ARG:HB3	1.58	0.43
1:B:146:VAL:HG13	1:B:148:LEU:HG	1.99	0.43
1:C:291:PRO:O	1:C:292:ILE:HB	2.18	0.43
1:B:103:GLN:HG3	1:B:407:LEU:HB3	2.00	0.43
1:B:214:LYS:HB3	1:B:214:LYS:HE3	1.84	0.43
1:C:75:ILE:HB	1:C:248:LEU:O	2.18	0.43
1:B:264:SER:OG	1:B:265:LYS:N	2.52	0.43
1:A:8:GLN:OE1	1:A:11:ARG:NH2	2.52	0.43
1:A:319:ALA:O	1:A:323:VAL:HG13	2.19	0.43
1:A:421:LYS:HA	1:A:422:PRO:HD3	1.93	0.43
1:C:235:GLU:OE2	1:C:238:ARG:NH1	2.52	0.43
1:A:75:ILE:HB	1:A:248:LEU:O	2.19	0.43
1:B:358:MSE:SE	1:B:367:ARG:HD2	2.69	0.43
1:A:18:ARG:HE	1:B:314:GLU:CD	2.26	0.42
1:C:24:ARG:NH1	2:C:764:HOH:O	2.52	0.42
1:C:197:ASN:ND2	1:C:200:ASN:H	2.17	0.42
1:A:358:MSE:SE	1:A:371:ASP:HB3	2.70	0.42
1:B:323:VAL:O	1:B:327:VAL:HG13	2.18	0.42
1:A:152:THR:CG2	2:B:432:HOH:O	2.67	0.42
1:C:250:LEU:C	1:C:250:LEU:HD23	2.43	0.42
1:A:47:ASP:HB3	1:B:287:SER:HA	2.00	0.42
1:C:55:ARG:O	1:C:56:ASP:HB3	2.20	0.42
1:A:330:SER:HB2	1:A:400:ILE:HG13	2.01	0.42
1:A:421:LYS:HG3	2:A:787:HOH:O	2.20	0.42
1:B:137:LEU:HD21	1:B:158:ARG:CZ	2.49	0.42
1:B:289:SER:HB2	2:B:775:HOH:O	2.20	0.42
1:C:365:GLY:HA2	2:C:543:HOH:O	2.18	0.42
1:B:160:GLN:HE21	1:B:160:GLN:HB2	1.42	0.42
1:B:320:HIS:CG	2:B:681:HOH:O	2.73	0.42
1:C:205:LYS:HD2	2:C:673:HOH:O	2.20	0.42
1:C:359:GLU:CD	2:C:526:HOH:O	2.62	0.42
1:A:42:LEU:HD12	1:A:70:GLN:O	2.19	0.42
1:A:46:ALA:HA	1:A:67:ALA:HA	2.01	0.42
1:B:86:LEU:HD13	1:B:235:GLU:CG	2.50	0.42
1:B:152:THR:CG2	2:C:431:HOH:O	2.67	0.42
1:B:270:ALA:HB1	1:B:274:TYR:CD2	2.55	0.42
1:C:54:TYR:O	2:C:695:HOH:O	2.22	0.42
1:C:86:LEU:HD13	1:C:235:GLU:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:THR:CG2	2:C:546:HOH:O	2.66	0.41
1:B:207:GLN:NE2	2:B:815:HOH:O	2.51	0.41
1:C:86:LEU:HD13	1:C:235:GLU:HG3	2.02	0.41
1:A:8:GLN:HG3	2:A:778:HOH:O	2.19	0.41
1:B:75:ILE:HG21	1:B:248:LEU:HD12	2.02	0.41
1:C:68:SER:HB3	1:C:255:GLY:HA3	2.02	0.41
1:A:80:LYS:HE2	2:A:570:HOH:O	2.20	0.41
1:A:166:ALA:HA	1:A:169:LEU:CD2	2.49	0.41
1:A:271:GLY:O	1:A:272:THR:HB	2.19	0.41
1:A:367:ARG:HH12	1:C:156:ASN:ND2	2.05	0.41
1:B:4:MSE:SE	2:B:704:HOH:O	2.88	0.41
1:A:54:TYR:O	1:A:55:ARG:C	2.64	0.41
1:A:223:LEU:C	1:A:223:LEU:HD12	2.45	0.41
1:A:263:GLY:O	1:A:264:SER:C	2.63	0.41
1:B:47:ASP:HB3	1:C:287:SER:HA	2.02	0.41
1:B:365:GLY:HA2	2:B:647:HOH:O	2.20	0.41
1:C:79:SER:CA	2:C:933:HOH:O	2.47	0.41
1:A:42:LEU:O	1:B:291:PRO:O	2.38	0.41
1:B:270:ALA:HB1	1:B:274:TYR:HD2	1.86	0.41
1:C:79:SER:HB2	2:C:933:HOH:O	2.21	0.41
1:C:223:LEU:HD11	2:C:873:HOH:O	2.20	0.41
1:C:274:TYR:CE2	2:C:896:HOH:O	2.57	0.41
1:C:82:ARG:HG2	1:C:239:GLN:HA	2.02	0.41
1:B:8:GLN:OE1	1:B:11:ARG:NH2	2.54	0.41
1:C:302:VAL:O	1:C:306:GLN:HG3	2.21	0.41
1:A:68:SER:HB3	1:A:255:GLY:HA3	2.02	0.41
1:A:219:ARG:CD	2:A:571:HOH:O	2.60	0.41
1:B:60:ILE:HD12	1:B:274:TYR:CE1	2.56	0.41
1:C:214:LYS:HB3	1:C:214:LYS:HE3	1.88	0.41
1:A:11:ARG:NH1	1:A:409:GLU:OE2	2.54	0.41
1:A:24:ARG:HE	1:A:24:ARG:HB3	1.61	0.41
1:A:291:PRO:O	1:C:42:LEU:O	2.39	0.41
1:A:294:GLN:HB3	1:C:41:GLN:NE2	2.36	0.41
2:A:547:HOH:O	1:C:170:THR:HG22	2.20	0.41
1:A:160:GLN:NE2	2:A:525:HOH:O	2.53	0.40
1:B:219:ARG:HB2	1:B:404:LEU:O	2.22	0.40
1:A:359:GLU:HB3	2:A:622:HOH:O	2.22	0.40
1:B:398:LEU:HD11	1:B:415:LEU:CD1	2.51	0.40
1:C:358:MSE:SE	1:C:367:ARG:NH1	2.99	0.40
1:A:197:ASN:HD22	1:A:197:ASN:C	2.29	0.40
1:B:75:ILE:HB	1:B:248:LEU:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:THR:HG23	2:B:803:HOH:O	2.20	0.40
1:C:32:ASN:ND2	1:C:35:ARG:HH22	2.15	0.40
1:A:84:LEU:O	1:A:88:GLU:HG3	2.22	0.40
1:B:388:ASN:CB	2:B:597:HOH:O	2.69	0.40

All (2) 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:773:HOH:O	2:C:709:HOH:O[9_554]	2.11	0.09
2:A:683:HOH:O	2:B:797:HOH:O[9_554]	2.15	0.05

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	426/428 (100%)	403 (95%)	19 (4%)	4 (1%)	14	10
1	B	426/428 (100%)	403 (95%)	19 (4%)	4 (1%)	14	10
1	C	426/428 (100%)	397 (93%)	25 (6%)	4 (1%)	14	10
All	All	1278/1284 (100%)	1203 (94%)	63 (5%)	12 (1%)	14	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	THR
1	B	279	MSE
1	A	259	THR
1	C	259	THR
1	C	279	MSE
1	A	55	ARG
1	A	279	MSE

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Mol	Chain	Res	Type
1	B	55	ARG
1	C	268	GLY
1	C	55	ARG
1	B	268	GLY
1	A	268	GLY

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	358/353 (101%)	314 (88%)	44 (12%)	4	2
1	B	358/353 (101%)	319 (89%)	39 (11%)	6	4
1	C	358/353 (101%)	310 (87%)	48 (13%)	4	2
All	All	1074/1059 (101%)	943 (88%)	131 (12%)	5	2

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	17	LEU
1	A	47	ASP
1	A	51	SER
1	A	60	ILE
1	A	65	THR
1	A	66	SER
1	A	71	LEU
1	A	79	SER
1	A	86	LEU
1	A	97	THR
1	A	139	GLN
1	A	152	THR
1	A	160	GLN
1	A	169	LEU
1	A	170	THR
1	A	186	THR

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Mol	Chain	Res	Type
1	A	197	ASN
1	A	199	GLU
1	A	200	ASN
1	A	202	LYS
1	A	217	GLU
1	A	223	LEU
1	A	247	THR
1	A	256	ILE
1	A	259	THR
1	A	262	SER
1	A	265	LYS
1	A	266	THR
1	A	272	THR
1	A	277	SER
1	A	279	MSE
1	A	281	GLN
1	A	290	LEU
1	A	310	VAL
1	A	316	LEU
1	A	323	VAL
1	A	327	VAL
1	A	397	GLN
1	A	398	LEU
1	A	400	ILE
1	A	401	LYS
1	A	407	LEU
1	A	412	LEU
1	B	12	LEU
1	B	17	LEU
1	B	51	SER
1	B	60	ILE
1	B	65	THR
1	B	66	SER
1	B	71	LEU
1	B	86	LEU
1	B	97	THR
1	B	152	THR
1	B	160	GLN
1	B	170	THR
1	B	186	THR
1	B	199	GLU
1	B	217	GLU

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Mol	Chain	Res	Type
1	B	223	LEU
1	B	247	THR
1	B	248	LEU
1	B	256	ILE
1	B	259	THR
1	B	262	SER
1	B	265	LYS
1	B	266	THR
1	B	272	THR
1	B	277	SER
1	B	279	MSE
1	B	281	GLN
1	B	290	LEU
1	B	310	VAL
1	B	316	LEU
1	B	323	VAL
1	B	327	VAL
1	B	353	SER
1	B	397	GLN
1	B	398	LEU
1	B	400	ILE
1	B	401	LYS
1	B	407	LEU
1	B	412	LEU
1	C	4	MSE
1	C	12	LEU
1	C	17	LEU
1	C	47	ASP
1	C	51	SER
1	C	60	ILE
1	C	65	THR
1	C	71	LEU
1	C	86	LEU
1	C	97	THR
1	C	139	GLN
1	C	146	VAL
1	C	149	VAL
1	C	152	THR
1	C	160	GLN
1	C	170	THR
1	C	186	THR
1	C	197	ASN

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Mol	Chain	Res	Type
1	C	199	GLU
1	C	200	ASN
1	C	202	LYS
1	C	217	GLU
1	C	223	LEU
1	C	232	LEU
1	C	247	THR
1	C	248	LEU
1	C	251	THR
1	C	256	ILE
1	C	259	THR
1	C	262	SER
1	C	265	LYS
1	C	266	THR
1	C	272	THR
1	C	277	SER
1	C	279	MSE
1	C	281	GLN
1	C	290	LEU
1	C	310	VAL
1	C	316	LEU
1	C	323	VAL
1	C	327	VAL
1	C	353	SER
1	C	397	GLN
1	C	398	LEU
1	C	400	ILE
1	C	401	LYS
1	C	407	LEU
1	C	412	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	41	GLN
1	A	52	ASN
1	A	73	GLN
1	A	103	GLN
1	A	108	ASN
1	A	115	ASN
1	A	118	ASN

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Mol	Chain	Res	Type
1	A	127	GLN
1	A	139	GLN
1	A	142	GLN
1	A	155	GLN
1	A	156	ASN
1	A	160	GLN
1	A	174	ASN
1	A	197	ASN
1	A	200	ASN
1	A	210	ASN
1	A	220	ASN
1	A	225	GLN
1	A	273	GLN
1	A	281	GLN
1	A	301	GLN
1	A	315	GLN
1	A	332	ASN
1	A	342	ASN
1	A	381	ASN
1	A	384	GLN
1	A	388	ASN
1	A	392	ASN
1	A	397	GLN
1	A	399	ASN
1	A	417	ASN
1	B	32	ASN
1	B	41	GLN
1	B	52	ASN
1	B	108	ASN
1	B	115	ASN
1	B	118	ASN
1	B	127	GLN
1	B	136	GLN
1	B	139	GLN
1	B	142	GLN
1	B	155	GLN
1	B	156	ASN
1	B	160	GLN
1	B	174	ASN
1	B	197	ASN
1	B	210	ASN
1	B	220	ASN

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Mol	Chain	Res	Type
1	B	225	GLN
1	B	273	GLN
1	B	281	GLN
1	B	301	GLN
1	B	315	GLN
1	B	342	ASN
1	B	346	GLN
1	B	388	ASN
1	B	392	ASN
1	B	397	GLN
1	B	399	ASN
1	B	417	ASN
1	C	32	ASN
1	C	41	GLN
1	C	52	ASN
1	C	87	GLN
1	C	108	ASN
1	C	115	ASN
1	C	118	ASN
1	C	139	GLN
1	C	155	GLN
1	C	156	ASN
1	C	160	GLN
1	C	174	ASN
1	C	197	ASN
1	C	200	ASN
1	C	210	ASN
1	C	220	ASN
1	C	281	GLN
1	C	299	ASN
1	C	301	GLN
1	C	332	ASN
1	C	342	ASN
1	C	381	ASN
1	C	388	ASN
1	C	392	ASN
1	C	397	GLN
1	C	399	ASN
1	C	417	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	423/428 (98%)	0.93	85 (20%) 3 3	25, 48, 81, 84	0
1	B	423/428 (98%)	1.06	82 (19%) 3 3	24, 47, 81, 84	0
1	C	423/428 (98%)	1.03	89 (21%) 2 2	24, 47, 81, 84	0
All	All	1269/1284 (98%)	1.01	256 (20%) 3 3	24, 47, 81, 84	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	274	TYR	8.8
1	B	264	SER	8.5
1	B	268	GLY	8.3
1	B	270	ALA	8.1
1	C	270	ALA	8.0
1	B	59	GLY	8.0
1	B	263	GLY	7.4
1	C	269	ALA	7.4
1	B	269	ALA	7.2
1	B	267	ARG	6.8
1	B	60	ILE	6.6
1	B	54	TYR	6.6
1	C	268	GLY	6.4
1	B	274	TYR	6.2
1	A	264	SER	6.1
1	C	271	GLY	6.0
1	C	266	THR	5.8
1	B	53	GLY	5.8
1	B	50	TYR	5.7
1	B	275	ASP	5.6
1	C	273	GLN	5.6
1	C	63	ASN	5.6
1	B	48	TYR	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	272	THR	5.4
1	C	262	SER	5.4
1	C	280	GLY	5.4
1	B	271	GLY	5.3
1	A	263	GLY	5.2
1	C	48	TYR	5.1
1	C	261	TYR	5.1
1	A	63	ASN	5.0
1	C	260	SER	4.9
1	B	266	THR	4.8
1	B	57	ALA	4.8
1	B	273	GLN	4.8
1	B	284	VAL	4.8
1	C	59	GLY	4.7
1	C	65	THR	4.7
1	C	256	ILE	4.6
1	C	263	GLY	4.6
1	A	267	ARG	4.6
1	C	267	ARG	4.5
1	B	63	ASN	4.5
1	C	428	GLU	4.4
1	C	169	LEU	4.4
1	C	54	TYR	4.4
1	B	1	GLU	4.4
1	B	189	TYR	4.3
1	B	61	ASN	4.3
1	C	281	GLN	4.3
1	B	256	ILE	4.2
1	C	60	ILE	4.1
1	A	65	THR	4.1
1	C	272	THR	4.1
1	B	262	SER	4.1
1	A	60	ILE	4.1
1	A	69	LEU	4.1
1	C	259	THR	4.1
1	B	280	GLY	4.0
1	C	67	ALA	4.0
1	C	255	GLY	4.0
1	B	58	ASN	4.0
1	B	169	LEU	4.0
1	C	257	SER	4.0
1	B	12	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	256	ILE	3.9
1	C	66	SER	3.9
1	B	46	ALA	3.9
1	C	142	GLN	3.8
1	A	271	GLY	3.8
1	A	46	ALA	3.8
1	C	275	ASP	3.8
1	A	48	TYR	3.8
1	C	57	ALA	3.8
1	B	65	THR	3.8
1	C	49	THR	3.8
1	C	1	GLU	3.8
1	C	64	ALA	3.7
1	C	278	ASN	3.6
1	A	284	VAL	3.6
1	A	52	ASN	3.6
1	A	250	LEU	3.6
1	A	278	ASN	3.6
1	C	50	TYR	3.6
1	A	62	SER	3.5
1	C	69	LEU	3.5
1	A	280	GLY	3.5
1	A	55	ARG	3.5
1	C	55	ARG	3.5
1	B	259	THR	3.5
1	A	64	ALA	3.5
1	A	169	LEU	3.5
1	A	200	ASN	3.4
1	A	259	THR	3.4
1	A	262	SER	3.4
1	B	69	LEU	3.4
1	B	52	ASN	3.4
1	A	254	THR	3.4
1	B	255	GLY	3.4
1	A	67	ALA	3.4
1	B	265	LYS	3.4
1	B	257	SER	3.4
1	C	283	LYS	3.3
1	A	223	LEU	3.3
1	C	56	ASP	3.3
1	C	139	GLN	3.3
1	A	57	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	50	TYR	3.2
1	B	64	ALA	3.2
1	C	286	LEU	3.2
1	C	265	LYS	3.2
1	C	146	VAL	3.2
1	A	292	ILE	3.2
1	B	286	LEU	3.2
1	C	264	SER	3.2
1	B	278	ASN	3.2
1	B	250	LEU	3.1
1	C	75	ILE	3.1
1	B	258	ASP	3.1
1	A	202	LYS	3.1
1	A	266	THR	3.1
1	C	53	GLY	3.1
1	B	42	LEU	3.1
1	B	71	LEU	3.1
1	A	59	GLY	3.1
1	A	49	THR	3.1
1	A	252	ALA	3.1
1	C	68	SER	3.0
1	A	281	GLN	3.0
1	A	248	LEU	3.0
1	C	282	ASN	3.0
1	C	254	THR	3.0
1	B	261	TYR	3.0
1	C	189	TYR	3.0
1	B	81	TRP	3.0
1	C	58	ASN	2.9
1	B	252	ALA	2.9
1	C	52	ASN	2.9
1	A	286	LEU	2.9
1	C	276	ASP	2.9
1	A	261	TYR	2.9
1	A	277	SER	2.9
1	A	285	GLY	2.9
1	B	248	LEU	2.8
1	A	257	SER	2.8
1	B	223	LEU	2.8
1	B	75	ILE	2.8
1	B	281	GLN	2.8
1	A	428	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	413	LEU	2.8
1	C	148	LEU	2.8
1	B	49	THR	2.8
1	A	420	SER	2.8
1	C	253	SER	2.8
1	A	54	TYR	2.8
1	C	223	LEU	2.8
1	B	428	GLU	2.7
1	C	295	GLY	2.7
1	C	62	SER	2.7
1	C	287	SER	2.7
1	C	47	ASP	2.7
1	C	38	LEU	2.7
1	C	71	LEU	2.7
1	A	237	ILE	2.7
1	B	260	SER	2.7
1	A	255	GLY	2.7
1	C	299	ASN	2.7
1	A	258	ASP	2.6
1	A	298	VAL	2.6
1	C	292	ILE	2.6
1	A	247	THR	2.6
1	A	245	LEU	2.6
1	C	412	LEU	2.6
1	A	269	ALA	2.6
1	B	44	LEU	2.6
1	B	295	GLY	2.6
1	A	32	ASN	2.6
1	A	282	ASN	2.6
1	B	38	LEU	2.6
1	B	39	LEU	2.6
1	C	248	LEU	2.6
1	C	8	GLN	2.5
1	B	62	SER	2.5
1	B	276	ASP	2.5
1	A	291	PRO	2.5
1	B	34	ALA	2.5
1	A	71	LEU	2.5
1	B	199	GLU	2.5
1	B	251	THR	2.5
1	C	12	LEU	2.5
1	B	288	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	47	ASP	2.4
1	A	274	TYR	2.4
1	A	260	SER	2.4
1	C	277	SER	2.4
1	A	61	ASN	2.4
1	B	221	LEU	2.4
1	A	268	GLY	2.4
1	C	147	GLY	2.4
1	C	388	ASN	2.4
1	A	287	SER	2.4
1	A	75	ILE	2.4
1	C	37	PRO	2.4
1	C	285	GLY	2.3
1	C	258	ASP	2.3
1	A	76	PHE	2.3
1	A	265	LYS	2.3
1	A	189	TYR	2.3
1	A	283	LYS	2.3
1	C	291	PRO	2.3
1	B	214	LYS	2.3
1	C	217	GLU	2.3
1	B	200	ASN	2.3
1	B	283	LYS	2.3
1	C	413	LEU	2.3
1	A	288	PHE	2.2
1	B	292	ILE	2.2
1	A	44	LEU	2.2
1	A	232	LEU	2.2
1	A	290	LEU	2.2
1	A	413	LEU	2.2
1	C	221	LEU	2.2
1	A	243	GLY	2.2
1	A	270	ALA	2.2
1	B	388	ASN	2.2
1	B	234	ARG	2.1
1	C	249	ASP	2.1
1	B	76	PHE	2.1
1	C	298	VAL	2.1
1	A	51	SER	2.1
1	B	51	SER	2.1
1	A	58	ASN	2.1
1	C	61	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	272	THR	2.1
1	B	85	THR	2.1
1	A	45	GLY	2.1
1	B	55	ARG	2.1
1	C	284	VAL	2.1
1	C	34	ALA	2.1
1	A	293	TYR	2.1
1	A	198	VAL	2.1
1	A	305	ALA	2.1
1	C	418	ALA	2.1
1	B	299	ASN	2.0
1	A	56	ASP	2.0
1	B	56	ASP	2.0
1	B	70	GLN	2.0
1	C	251	THR	2.0
1	A	146	VAL	2.0
1	C	76	PHE	2.0
1	A	74	SER	2.0
1	B	67	ALA	2.0
1	C	81	TRP	2.0
1	A	12	LEU	2.0
1	A	38	LEU	2.0
1	A	246	PRO	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.