



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:57 AM UTC

PDB ID : 2FSF / pdb_00002fsf
Title : Escherichia coli SecA, the preprotein translocase dimeric ATPase
Authors : Papanikolau, Y.; Petratos, K.; Economou, A.
Deposited on : 2006-01-23
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

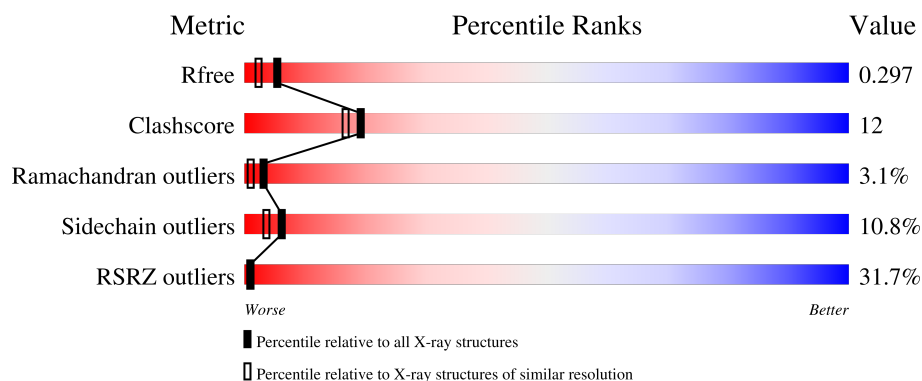
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	853	
1	B	853	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11637 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 Preprotein translocase secA subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5462	3426	966	1044	26			
1	B	723	Total	C	N	O	S	0	0	0
			5741	3600	1009	1104	28			

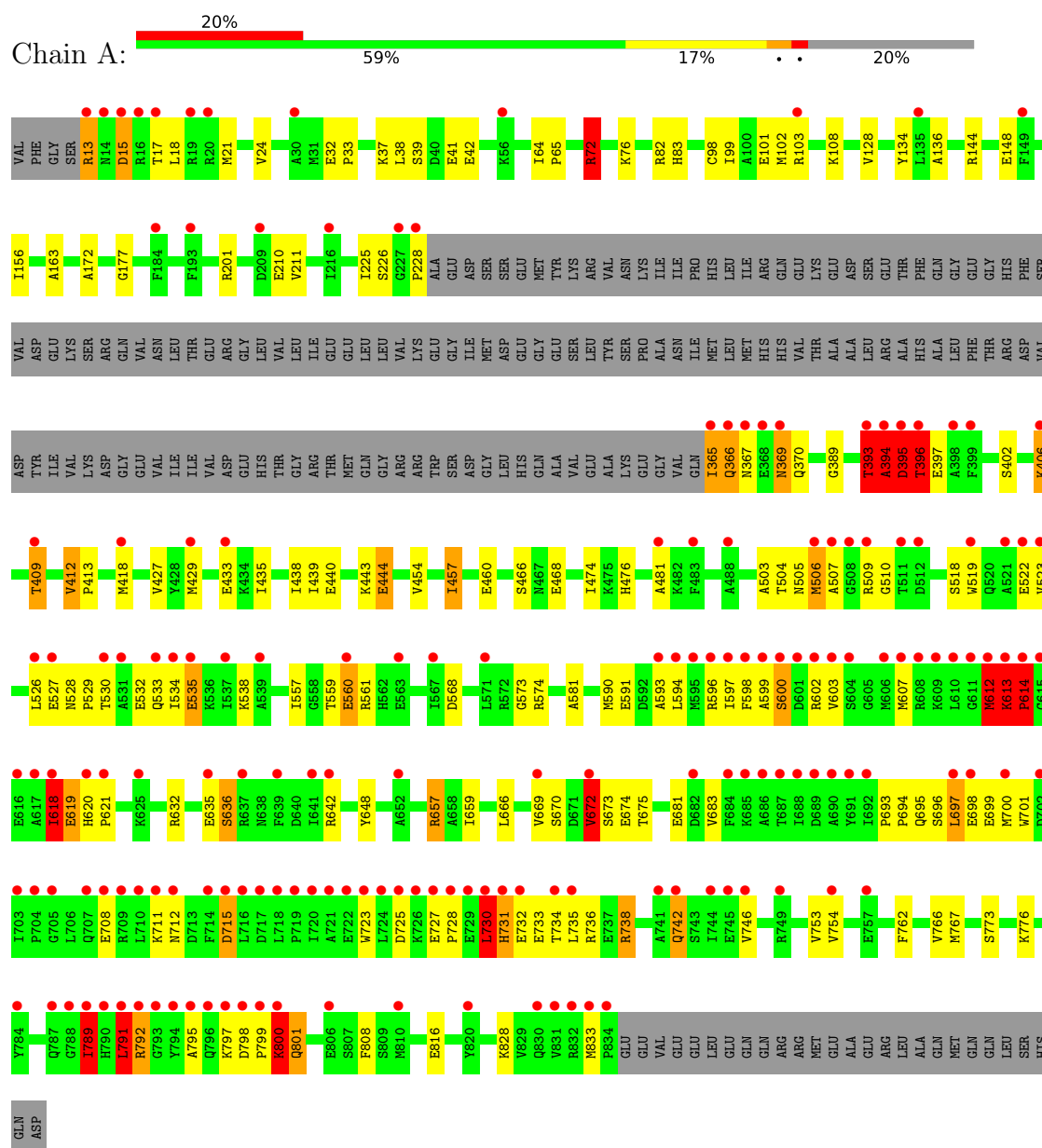
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total	O	0	0
			177	177		
2	B	257	Total	O	0	0
			257	257		

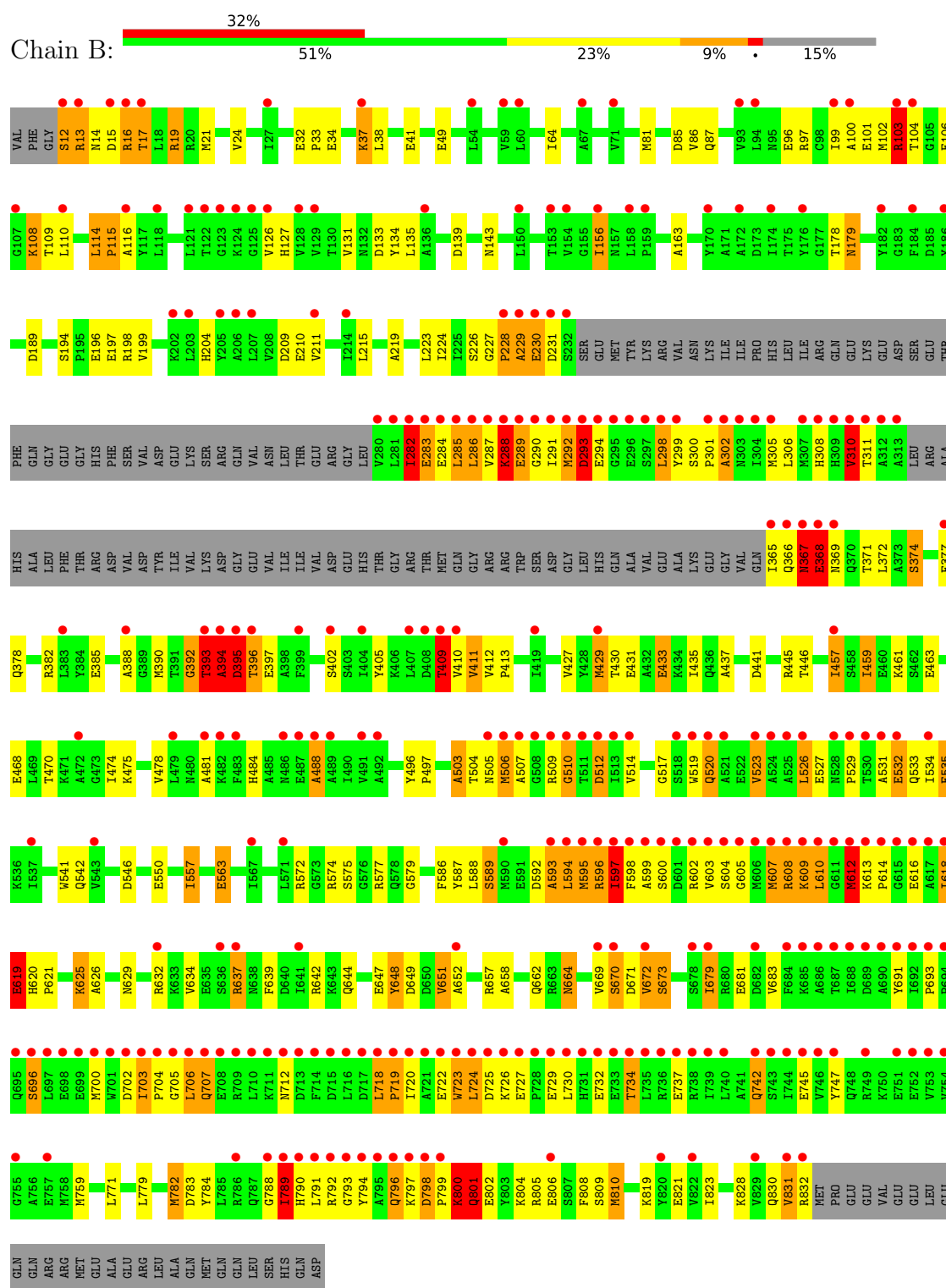
3 Residue-property plots

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: Preprotein translocase secA subunit



- Molecule 1: Preprotein translocase secA subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.03Å 90.17Å 163.05Å 90.00° 100.48° 90.00°	Depositor
Resolution (Å)	19.98 – 2.00 19.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.98-2.00) 97.0 (19.98-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.261 0.260 , 0.297	Depositor DCC
R_{free} test set	7010 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11637	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.61	44/5552 (0.8%)	1.34	29/7491 (0.4%)
1	B	1.84	95/5833 (1.6%)	1.48	63/7870 (0.8%)
All	All	1.73	139/11385 (1.2%)	1.41	92/15361 (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	4
1	B	0	9
All	All	0	13

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	LEU	C-N	14.88	1.56	1.33
1	B	393	THR	N-CA	13.38	1.63	1.46
1	B	395	ASP	N-CA	13.01	1.62	1.46
1	B	64	ILE	CA-CB	12.69	1.61	1.54
1	A	698	GLU	C-O	11.84	1.39	1.24
1	B	393	THR	C-O	11.39	1.38	1.24
1	A	163	ALA	CA-CB	-10.85	1.39	1.53
1	B	114	LEU	C-O	-10.68	1.15	1.24
1	B	652	ALA	CA-CB	10.61	1.69	1.53
1	B	395	ASP	CA-C	10.13	1.66	1.52
1	B	801	GLN	N-CA	9.97	1.59	1.46
1	A	698	GLU	C-N	9.86	1.47	1.33
1	B	394	ALA	CA-C	9.79	1.65	1.52
1	B	393	THR	CA-CB	9.01	1.68	1.53
1	B	32	GLU	C-O	-9.00	1.16	1.24
1	B	127	HIS	C-O	-8.92	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	695	GLN	C-O	8.40	1.39	1.24
1	A	396	THR	N-CA	8.38	1.57	1.46
1	B	126	VAL	C-O	-8.23	1.15	1.24
1	B	405	TYR	CA-C	-8.11	1.41	1.52
1	A	466	SER	C-O	8.06	1.33	1.24
1	A	136	ALA	CA-CB	8.02	1.65	1.53
1	B	13	ARG	CA-C	7.96	1.57	1.52
1	B	831	VAL	CA-CB	7.88	1.64	1.54
1	B	194	SER	C-O	-7.82	1.16	1.24
1	A	801	GLN	N-CA	7.78	1.56	1.46
1	A	698	GLU	CD-OE2	7.74	1.40	1.25
1	A	395	ASP	CA-C	7.67	1.63	1.52
1	B	109	THR	N-CA	-7.55	1.37	1.46
1	B	131	VAL	CA-C	-7.42	1.42	1.52
1	B	651	VAL	CA-CB	-7.38	1.45	1.54
1	B	626	ALA	CA-CB	-7.36	1.41	1.53
1	B	393	THR	CA-C	7.11	1.62	1.52
1	B	789	ILE	CA-CB	7.08	1.64	1.54
1	B	103	ARG	CG-CD	6.91	1.73	1.52
1	B	394	ALA	CA-CB	6.86	1.65	1.53
1	B	85	ASP	N-CA	-6.81	1.38	1.46
1	B	503	ALA	CA-CB	-6.80	1.41	1.53
1	B	474	ILE	C-O	6.75	1.31	1.24
1	B	101	GLU	C-N	-6.69	1.25	1.33
1	B	24	VAL	CA-CB	-6.68	1.45	1.54
1	B	100	ALA	CA-CB	6.68	1.61	1.53
1	A	98	CYS	CB-SG	-6.65	1.59	1.81
1	B	134	TYR	CA-C	6.59	1.61	1.52
1	B	163	ALA	CA-CB	6.57	1.62	1.53
1	A	697	LEU	CA-C	6.55	1.62	1.53
1	A	427	VAL	CA-CB	6.50	1.62	1.54
1	A	698	GLU	CD-OE1	6.44	1.37	1.25
1	B	801	GLN	CA-C	-6.44	1.44	1.52
1	A	697	LEU	C-O	6.41	1.32	1.23
1	B	468	GLU	C-O	-6.37	1.16	1.24
1	A	394	ALA	CA-CB	6.25	1.64	1.53
1	A	438	ILE	CA-CB	-6.24	1.47	1.54
1	B	49	GLU	CA-C	6.23	1.60	1.52
1	A	454	VAL	CA-CB	-6.23	1.46	1.54
1	B	392	GLY	N-CA	6.16	1.52	1.45
1	B	435	ILE	C-O	-6.12	1.17	1.24
1	A	64	ILE	C-O	-6.06	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	672	VAL	CA-CB	6.05	1.62	1.54
1	B	156	ILE	C-O	-6.05	1.17	1.24
1	B	427	VAL	CA-C	-6.03	1.45	1.52
1	B	669	VAL	CA-C	6.02	1.59	1.52
1	B	179	ASN	C-O	5.98	1.30	1.24
1	A	670	SER	N-CA	5.97	1.54	1.46
1	A	612	MET	CA-C	5.91	1.60	1.52
1	B	390	MET	SD-CE	-5.91	1.64	1.79
1	A	394	ALA	C-O	5.91	1.31	1.24
1	B	86	VAL	N-CA	5.90	1.54	1.46
1	B	209	ASP	C-O	5.86	1.31	1.24
1	A	177	GLY	C-O	-5.86	1.17	1.24
1	B	199	VAL	N-CA	5.86	1.52	1.45
1	B	311	THR	CA-CB	5.84	1.62	1.53
1	B	87	GLN	N-CA	-5.80	1.39	1.46
1	B	808	PHE	C-O	-5.79	1.16	1.24
1	B	410	VAL	C-O	-5.75	1.17	1.24
1	B	116	ALA	N-CA	-5.74	1.39	1.46
1	B	658	ALA	CA-CB	-5.74	1.44	1.53
1	A	659	ILE	CA-CB	5.73	1.61	1.54
1	A	163	ALA	C-O	-5.73	1.19	1.24
1	B	310	VAL	CA-CB	5.71	1.62	1.54
1	B	395	ASP	C-O	5.71	1.31	1.24
1	A	560	GLU	CG-CD	5.71	1.66	1.52
1	B	470	THR	CA-C	-5.71	1.45	1.52
1	B	388	ALA	CA-CB	5.70	1.63	1.53
1	B	648	TYR	CA-C	-5.70	1.45	1.52
1	B	586	PHE	CA-C	-5.65	1.45	1.52
1	B	284	GLU	CD-OE2	5.64	1.36	1.25
1	A	559	THR	CA-CB	5.60	1.62	1.53
1	B	413	PRO	C-O	5.60	1.30	1.23
1	A	557	ILE	CA-CB	-5.59	1.47	1.54
1	B	197	GLU	C-O	-5.58	1.16	1.24
1	A	476	HIS	N-CA	-5.56	1.39	1.46
1	A	474	ILE	CA-CB	5.53	1.60	1.53
1	A	211	VAL	CA-CB	-5.53	1.46	1.54
1	A	792	ARG	N-CA	5.50	1.53	1.46
1	B	662	GLN	N-CA	-5.49	1.39	1.46
1	B	478	VAL	C-O	-5.49	1.16	1.24
1	B	390	MET	CA-C	-5.48	1.46	1.52
1	B	178	THR	CA-CB	5.47	1.62	1.53
1	B	664	ASN	C-O	5.47	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	512	ASP	CB-CG	5.45	1.65	1.52
1	B	412	VAL	CA-C	5.44	1.57	1.53
1	B	101	GLU	CA-C	5.43	1.59	1.52
1	B	619	GLU	N-CA	5.43	1.53	1.46
1	B	204	HIS	C-O	-5.41	1.17	1.23
1	A	172	ALA	CA-CB	-5.41	1.45	1.53
1	B	433	GLU	C-O	-5.41	1.17	1.24
1	B	618	ILE	CA-C	5.39	1.59	1.52
1	A	418	MET	SD-CE	5.37	1.93	1.79
1	A	389	GLY	C-O	-5.35	1.18	1.23
1	B	809	SER	N-CA	-5.32	1.39	1.46
1	B	670	SER	N-CA	5.31	1.53	1.46
1	B	402	SER	CA-C	5.26	1.59	1.52
1	B	557	ILE	CA-CB	-5.25	1.48	1.54
1	B	97	ARG	CG-CD	5.24	1.68	1.52
1	B	802	GLU	C-O	-5.24	1.17	1.24
1	A	791	LEU	CA-C	5.24	1.59	1.52
1	B	115	PRO	N-CA	5.23	1.54	1.47
1	B	395	ASP	CA-CB	5.22	1.62	1.53
1	B	802	GLU	C-N	5.21	1.40	1.33
1	A	481	ALA	CA-CB	5.19	1.62	1.53
1	B	17	THR	CA-CB	5.18	1.61	1.53
1	B	133	ASP	N-CA	-5.17	1.39	1.46
1	B	672	VAL	CA-CB	5.16	1.61	1.54
1	B	189	ASP	C-O	-5.15	1.17	1.24
1	B	488	ALA	CA-CB	-5.15	1.44	1.53
1	A	581	ALA	CA-C	5.13	1.59	1.52
1	A	134	TYR	CA-C	5.09	1.59	1.52
1	B	41	GLU	CA-C	5.09	1.59	1.52
1	B	143	ASN	CA-C	-5.08	1.45	1.52
1	B	649	ASP	CA-C	5.07	1.59	1.52
1	B	810	MET	C-O	-5.06	1.18	1.24
1	B	588	LEU	CA-C	-5.06	1.46	1.52
1	B	475	LYS	CA-C	-5.05	1.46	1.52
1	B	512	ASP	CA-C	5.04	1.59	1.52
1	A	393	THR	CA-CB	5.03	1.61	1.53
1	A	808	PHE	C-O	-5.03	1.18	1.24
1	B	625	LYS	CD-CE	5.02	1.67	1.52
1	A	683	VAL	CA-CB	5.01	1.60	1.54

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	LYS	CA-C-N	10.33	132.76	119.84
1	A	613	LYS	C-N-CA	10.33	132.76	119.84
1	A	800	LYS	N-CA-C	-9.18	91.25	110.80
1	B	608	ARG	N-CA-C	-8.89	101.53	111.14
1	B	435	ILE	N-CA-C	-8.75	102.33	110.82
1	B	790	HIS	N-CA-C	-7.79	103.62	113.43
1	B	374	SER	CA-CB-OG	-7.71	95.69	111.10
1	B	801	GLN	N-CA-CB	7.56	123.27	110.49
1	B	34	GLU	CB-CA-C	-7.56	99.01	110.88
1	A	697	LEU	CA-C-N	-7.27	108.41	121.14
1	A	697	LEU	C-N-CA	-7.27	108.41	121.14
1	B	613	LYS	CA-C-N	7.26	128.91	119.84
1	B	613	LYS	C-N-CA	7.26	128.91	119.84
1	A	600	SER	N-CA-C	7.24	120.19	108.32
1	B	800	LYS	O-C-N	-7.13	114.44	122.86
1	B	210	GLU	CB-CA-C	-7.12	101.11	111.23
1	B	608	ARG	N-CA-CB	6.94	120.13	110.07
1	B	392	GLY	N-CA-C	6.92	119.95	112.33
1	A	674	GLU	N-CA-C	-6.87	103.72	111.07
1	B	800	LYS	CA-C-N	-6.80	108.55	121.54
1	B	800	LYS	C-N-CA	-6.80	108.55	121.54
1	B	445	ARG	N-CA-C	6.67	118.64	111.36
1	A	618	ILE	CB-CA-C	6.59	116.92	111.05
1	A	581	ALA	N-CA-C	-6.54	101.45	110.35
1	A	636	SER	N-CA-C	6.51	118.04	111.07
1	A	697	LEU	N-CA-C	-6.48	102.15	110.19
1	B	730	LEU	N-CA-C	6.47	119.15	111.71
1	A	698	GLU	O-C-N	6.41	131.31	122.46
1	A	715	ASP	N-CA-C	-6.40	104.77	112.58
1	B	13	ARG	N-CA-C	6.32	118.91	108.48
1	A	681	GLU	N-CA-C	-6.32	103.92	111.69
1	B	639	PHE	N-CA-C	6.31	118.96	111.71
1	A	753	VAL	N-CA-C	6.28	117.06	110.72
1	B	794	TYR	N-CA-C	6.23	124.06	110.80
1	B	563	GLU	N-CA-C	-6.22	104.50	111.28
1	B	108	LYS	N-CA-C	6.19	118.82	111.33
1	B	446	THR	N-CA-C	-6.12	104.69	111.36
1	B	228	PRO	N-CA-C	-6.09	105.06	113.53
1	A	72	ARG	NE-CZ-NH2	6.04	124.64	119.20
1	B	517	GLY	N-CA-C	-6.00	105.07	112.33
1	B	579	GLY	N-CA-C	5.99	123.32	115.47
1	B	723	TRP	N-CA-C	-5.96	104.47	110.97
1	B	819	LYS	N-CA-C	5.96	118.29	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	732	GLU	N-CA-C	5.92	117.73	111.28
1	A	673	SER	N-CA-C	5.92	123.40	110.80
1	B	437	ALA	N-CA-C	-5.91	104.42	111.69
1	B	394	ALA	N-CA-C	5.87	123.31	110.80
1	B	103	ARG	N-CA-C	5.86	118.51	110.24
1	B	474	ILE	N-CA-C	5.85	116.22	107.51
1	B	366	GLN	N-CA-C	5.80	120.51	112.45
1	A	712	ASN	N-CA-C	5.79	117.26	111.07
1	A	614	PRO	N-CA-C	5.78	124.38	112.47
1	A	412	VAL	CA-C-N	5.70	125.70	119.89
1	A	412	VAL	C-N-CA	5.70	125.70	119.89
1	B	681	GLU	N-CA-C	-5.70	104.99	111.14
1	B	517	GLY	CA-C-O	-5.67	118.04	122.52
1	A	568	ASP	N-CA-C	-5.65	105.20	111.36
1	B	412	VAL	CA-C-N	-5.60	114.48	120.03
1	B	412	VAL	C-N-CA	-5.60	114.48	120.03
1	B	806	GLU	N-CA-C	-5.50	105.29	112.23
1	B	411	VAL	CB-CA-C	-5.50	104.26	111.25
1	B	673	SER	CB-CA-C	-5.49	102.02	110.81
1	B	139	ASP	N-CA-C	5.46	116.91	111.07
1	B	395	ASP	N-CA-C	5.41	122.32	110.80
1	B	135	LEU	N-CA-C	5.39	117.15	111.28
1	B	672	VAL	N-CA-CB	-5.37	104.25	112.15
1	B	293	ASP	N-CA-C	5.37	122.23	110.80
1	A	698	GLU	N-CA-C	-5.37	106.24	112.89
1	B	669	VAL	CB-CA-C	5.37	118.97	110.81
1	B	572	ARG	CG-CD-NE	-5.33	100.27	112.00
1	A	210	GLU	CB-CA-C	-5.32	103.68	111.23
1	B	311	THR	N-CA-CB	5.32	118.41	110.22
1	B	782	MET	CG-SD-CE	5.32	112.59	100.90
1	B	392	GLY	CA-C-N	5.29	131.64	121.54
1	B	392	GLY	C-N-CA	5.29	131.64	121.54
1	B	393	THR	CA-C-O	5.28	128.06	120.51
1	B	103	ARG	CG-CD-NE	5.25	123.54	112.00
1	A	657	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	B	616	GLU	N-CA-C	5.22	116.66	110.19
1	B	367	ASN	N-CA-C	5.22	121.91	110.80
1	B	409	THR	N-CA-CB	5.19	118.72	110.57
1	A	574	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	B	642	ARG	N-CA-C	5.17	116.92	111.28
1	A	128	VAL	N-CA-C	-5.16	101.16	108.58
1	A	369	ASN	N-CA-C	5.14	117.00	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ARG	N-CA-C	5.11	116.54	111.07
1	B	282	ILE	CB-CA-C	-5.08	105.38	112.04
1	B	106	GLU	N-CA-C	5.06	119.43	113.16
1	B	429	MET	CG-SD-CE	-5.05	89.78	100.90
1	B	798	ASP	CA-C-N	5.05	124.50	119.24
1	B	798	ASP	C-N-CA	5.05	124.50	119.24
1	A	72	ARG	NE-CZ-NH1	-5.01	116.49	121.50

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Peptide
1	A	393	THR	Peptide
1	A	395	ASP	Peptide
1	A	697	LEU	Mainchain
1	B	229	ALA	Peptide
1	B	300	SER	Peptide
1	B	365	ILE	Peptide
1	B	393	THR	Peptide
1	B	394	ALA	Peptide
1	B	597	ILE	Peptide
1	B	607	MET	Peptide
1	B	610	LEU	Peptide
1	B	793	GLY	Peptide

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	5462	0	5460	95	0
1	B	5741	0	5731	167	1
2	A	177	0	0	12	0
2	B	257	0	0	29	0
All	All	11637	0	11191	262	1

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 12.

All (262) 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:96:GLU:HG3	2:B:1033:HOH:O	1.46	1.13
1:A:799:PRO:HA	2:A:1026:HOH:O	1.50	1.08
1:B:800:LYS:O	1:B:801:GLN:HB2	1.61	1.01
1:A:799:PRO:C	1:A:800:LYS:O	1.95	0.97
1:B:103:ARG:HG3	1:B:103:ARG:HH11	1.26	0.97
1:A:394:ALA:HA	2:A:980:HOH:O	1.68	0.92
1:A:15:ASP:HA	1:A:18:LEU:HB2	1.53	0.91
1:B:457:ILE:O	1:B:505:ASN:ND2	2.10	0.85
1:A:732:GLU:OE2	1:A:736:ARG:NH1	2.11	0.84
1:A:736:ARG:CZ	2:A:1005:HOH:O	2.25	0.84
1:A:799:PRO:CA	2:A:1026:HOH:O	2.18	0.82
1:A:731:HIS:HB3	2:A:1016:HOH:O	1.80	0.81
1:A:736:ARG:NE	2:A:1005:HOH:O	2.14	0.80
1:B:693:PRO:O	1:B:696:SER:HB2	1.80	0.80
1:A:598:PHE:O	1:A:600:SER:N	2.15	0.80
1:B:103:ARG:HD2	1:B:104:THR:N	1.99	0.78
1:A:535:GLU:OE1	1:A:535:GLU:HA	1.82	0.78
1:B:230:GLU:OE2	1:B:369:ASN:HA	1.85	0.77
1:B:395:ASP:CB	2:B:964:HOH:O	2.32	0.76
1:B:395:ASP:CA	2:B:964:HOH:O	2.34	0.76
1:A:102:MET:HE3	1:A:108:LYS:HG2	1.67	0.76
1:A:731:HIS:NE2	1:A:733:GLU:HB3	2.01	0.75
1:B:800:LYS:O	1:B:801:GLN:CB	2.23	0.75
1:B:33:PRO:O	1:B:37:LYS:HD3	1.86	0.74
1:A:103:ARG:NH1	1:A:573:GLY:O	2.21	0.74
1:B:17:THR:HG22	1:B:21:MET:HE2	1.69	0.74
1:B:103:ARG:HH11	1:B:103:ARG:CG	2.01	0.74
1:B:598:PHE:O	1:B:600:SER:N	2.21	0.73
1:B:788:GLY:O	1:B:792:ARG:N	2.21	0.72
1:B:16:ARG:NE	1:B:19:ARG:HH21	1.88	0.71
1:B:395:ASP:HB2	2:B:964:HOH:O	1.88	0.71
1:B:395:ASP:HA	2:B:964:HOH:O	1.89	0.71
1:B:608:ARG:HG3	2:B:1078:HOH:O	1.92	0.70
1:B:392:GLY:O	1:B:394:ALA:CA	2.40	0.70
1:B:228:PRO:O	1:B:230:GLU:N	2.23	0.69
1:A:657:ARG:HD3	2:A:1006:HOH:O	1.92	0.68
1:B:629:ASN:HD22	1:B:632:ARG:NH2	1.90	0.68
1:B:103:ARG:HD3	2:B:888:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLU:OE2	1:A:393:THR:HA	1.93	0.68
1:A:833:MET:HE2	1:A:833:MET:HA	1.76	0.68
1:B:103:ARG:HG3	1:B:103:ARG:NH1	2.05	0.67
1:A:72:ARG:HD2	1:A:82:ARG:HG2	1.75	0.67
1:B:179:ASN:CG	2:B:1017:HOH:O	2.37	0.66
1:A:530:THR:H	1:A:533:GLN:HE21	1.44	0.65
1:B:805:ARG:NE	2:B:1115:HOH:O	2.17	0.65
1:B:481:ALA:O	1:B:484:HIS:NE2	2.29	0.65
1:A:800:LYS:N	2:A:1026:HOH:O	2.30	0.65
1:A:594:LEU:C	1:A:596:ARG:H	2.05	0.65
1:B:520:GLN:H	1:B:520:GLN:HE21	1.44	0.65
1:B:718:LEU:O	1:B:720:ILE:N	2.30	0.65
1:B:14:ASN:ND2	2:B:1083:HOH:O	2.28	0.64
1:B:14:ASN:HB3	2:B:1083:HOH:O	1.97	0.63
1:B:504:THR:O	1:B:505:ASN:C	2.41	0.63
1:A:742:GLN:HE21	1:A:742:GLN:N	1.97	0.62
1:B:227:GLY:HA3	1:B:372:LEU:HD11	1.80	0.62
1:B:282:ILE:HD12	1:B:286:LEU:CD1	2.30	0.62
1:B:703:ILE:HA	1:B:706:LEU:HB3	1.82	0.62
1:B:718:LEU:O	1:B:720:ILE:HG13	1.99	0.61
1:B:459:ILE:O	1:B:463:GLU:HG3	2.00	0.61
1:A:395:ASP:CG	1:A:396:THR:N	2.58	0.61
1:B:104:THR:OG1	1:B:509:ARG:NE	2.33	0.61
1:B:529:PRO:HA	1:B:533:GLN:NE2	2.16	0.61
1:B:609:LYS:HB3	2:B:1050:HOH:O	1.99	0.60
1:B:594:LEU:C	1:B:596:ARG:H	2.08	0.60
1:B:771:LEU:C	1:B:771:LEU:HD23	2.26	0.60
1:B:385:GLU:OE2	2:B:1026:HOH:O	2.16	0.60
1:B:597:ILE:HD12	1:B:634:VAL:HG21	1.84	0.59
1:A:429:MET:HB2	1:A:433:GLU:OE2	2.03	0.59
1:B:563:GLU:HG3	1:B:597:ILE:HD13	1.84	0.59
1:B:503:ALA:HB1	1:B:506:MET:HG3	1.84	0.59
1:B:789:ILE:HG22	1:B:789:ILE:O	2.03	0.58
1:B:395:ASP:C	2:B:921:HOH:O	2.46	0.58
1:B:618:ILE:HG22	1:B:619:GLU:N	2.19	0.58
1:A:731:HIS:NE2	1:A:733:GLU:CB	2.66	0.58
1:A:614:PRO:HA	2:A:1024:HOH:O	2.04	0.58
1:B:293:ASP:N	1:B:293:ASP:OD2	2.36	0.57
1:B:496:TYR:CD2	1:B:497:PRO:HD2	2.40	0.57
1:A:530:THR:H	1:A:533:GLN:NE2	2.02	0.57
1:A:736:ARG:NH2	2:A:1005:HOH:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:GLY:O	1:B:394:ALA:N	2.37	0.57
1:B:430:THR:OG1	2:B:1099:HOH:O	2.18	0.57
1:B:103:ARG:HD2	1:B:104:THR:H	1.70	0.56
1:A:732:GLU:OE2	1:A:736:ARG:CZ	2.52	0.56
1:B:179:ASN:OD1	2:B:1017:HOH:O	2.17	0.56
1:B:706:LEU:C	1:B:706:LEU:HD12	2.30	0.56
1:B:223:LEU:HD21	1:B:377:PHE:CZ	2.41	0.56
1:B:378:GLN:O	1:B:382:ARG:HG3	2.04	0.56
1:B:104:THR:HG21	1:B:577:ARG:CZ	2.36	0.56
1:A:534:ILE:HG22	1:A:534:ILE:O	2.06	0.56
1:B:629:ASN:ND2	1:B:632:ARG:NH2	2.54	0.55
1:B:608:ARG:CG	2:B:1078:HOH:O	2.53	0.55
1:B:429:MET:HB3	1:B:433:GLU:OE2	2.06	0.55
1:B:282:ILE:HD11	1:B:298:LEU:HB3	1.88	0.55
1:B:290:GLY:HA2	1:B:293:ASP:HB3	1.89	0.55
1:B:703:ILE:O	1:B:705:GLY:N	2.40	0.54
1:A:738:ARG:O	1:A:742:GLN:NE2	2.40	0.54
1:B:619:GLU:N	2:B:1103:HOH:O	2.20	0.54
1:B:603:VAL:HG12	1:B:603:VAL:O	2.07	0.54
1:B:81:MET:HE2	1:B:110:LEU:HD22	1.90	0.54
1:A:435:ILE:HG21	1:A:468:GLU:HG3	1.89	0.53
1:A:789:ILE:HG23	1:A:789:ILE:O	2.08	0.53
1:B:488:ALA:O	2:B:1101:HOH:O	2.19	0.53
1:B:301:PRO:O	1:B:302:ALA:CB	2.56	0.53
1:A:799:PRO:C	2:A:1026:HOH:O	2.46	0.53
1:B:526:LEU:HD22	1:B:533:GLN:HE22	1.74	0.53
1:B:747:TYR:OH	1:B:759:MET:HE2	2.09	0.53
1:A:618:ILE:O	1:A:619:GLU:HB2	2.08	0.53
1:B:703:ILE:HG22	1:B:707:GLN:HG2	1.92	0.52
1:A:530:THR:HG1	1:A:533:GLN:H	1.56	0.52
1:B:782:MET:HE3	1:B:810:MET:HE2	1.91	0.52
1:A:440:GLU:O	1:A:444:GLU:CG	2.58	0.52
1:A:429:MET:HG2	1:A:612:MET:SD	2.49	0.52
1:A:798:ASP:OD1	1:A:799:PRO:O	2.28	0.52
1:B:607:MET:HB3	1:B:612:MET:CE	2.40	0.52
1:B:288:LYS:HG3	1:B:289:GLU:HG2	1.90	0.52
1:B:531:ALA:O	1:B:535:GLU:OE1	2.28	0.52
1:B:647:GLU:OE2	1:B:800:LYS:CE	2.59	0.51
1:A:519:TRP:HA	1:A:522:GLU:OE1	2.11	0.51
1:A:730:LEU:O	1:A:731:HIS:ND1	2.42	0.51
1:A:696:SER:HB2	1:A:700:MET:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:GLU:OE2	1:B:800:LYS:HE2	2.11	0.51
1:B:679:ILE:O	1:B:683:VAL:HG23	2.11	0.51
1:B:282:ILE:O	1:B:286:LEU:HB2	2.11	0.50
1:B:691:TYR:HB3	1:B:702:ASP:O	2.12	0.50
1:A:457:ILE:HG23	1:A:560:GLU:HB2	1.93	0.50
1:B:506:MET:HG2	2:B:983:HOH:O	2.12	0.50
1:A:594:LEU:O	1:A:597:ILE:HG12	2.11	0.50
1:B:282:ILE:HD12	1:B:286:LEU:HD13	1.93	0.50
1:B:589:SER:HB2	1:B:592:ASP:OD2	2.11	0.50
1:A:395:ASP:O	1:A:397:GLU:OE2	2.29	0.50
1:B:16:ARG:NE	1:B:19:ARG:NH2	2.57	0.50
1:B:507:ALA:N	2:B:983:HOH:O	2.30	0.50
1:B:712:ASN:C	1:B:828:LYS:HZ1	2.18	0.50
1:B:114:LEU:HB2	1:B:115:PRO:CD	2.41	0.50
1:B:395:ASP:HB2	2:B:892:HOH:O	2.11	0.49
1:B:520:GLN:H	1:B:520:GLN:NE2	2.09	0.49
1:A:32:GLU:HB3	1:A:33:PRO:HD3	1.94	0.49
1:A:39:SER:OG	1:A:42:GLU:HG3	2.12	0.49
1:A:144:ARG:CG	1:A:148:GLU:OE1	2.61	0.48
1:A:457:ILE:HA	1:A:505:ASN:OD1	2.12	0.48
1:A:394:ALA:O	1:A:396:THR:N	2.45	0.48
1:B:532:GLU:HA	1:B:535:GLU:HB2	1.95	0.48
1:A:144:ARG:HG2	1:A:148:GLU:OE1	2.13	0.48
1:A:590:MET:SD	1:A:607:MET:HB2	2.53	0.48
1:B:395:ASP:C	1:B:397:GLU:H	2.21	0.48
1:B:16:ARG:HE	1:B:19:ARG:NH2	2.12	0.48
1:B:102:MET:HE3	1:B:108:LYS:HG2	1.96	0.48
1:B:679:ILE:CG1	1:B:823:ILE:HD11	2.44	0.48
1:B:395:ASP:HA	2:B:1077:HOH:O	2.14	0.48
1:A:402:SER:O	1:A:406:LYS:HD3	2.14	0.47
1:A:800:LYS:NZ	1:A:800:LYS:HB3	2.28	0.47
1:A:99:ILE:HB	1:A:409:THR:HB	1.96	0.47
1:A:675:THR:HG21	1:A:767:MET:HE1	1.95	0.47
1:B:519:TRP:HB3	1:B:541:TRP:CG	2.49	0.47
1:A:594:LEU:C	1:A:596:ARG:N	2.71	0.47
1:B:301:PRO:O	1:B:302:ALA:HB2	2.13	0.47
1:A:435:ILE:O	1:A:439:ILE:HG12	2.13	0.47
1:A:440:GLU:O	1:A:444:GLU:HG3	2.14	0.47
1:B:228:PRO:O	1:B:230:GLU:OE2	2.31	0.47
1:B:529:PRO:HA	1:B:533:GLN:HE21	1.79	0.47
1:A:742:GLN:O	1:A:746:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:SER:HB2	1:B:15:ASP:OD1	2.15	0.47
1:B:607:MET:HB3	1:B:612:MET:HE1	1.97	0.47
1:B:651:VAL:CG2	1:B:804:LYS:HG2	2.45	0.47
1:B:282:ILE:HD12	1:B:286:LEU:HD12	1.97	0.46
1:B:308:HIS:CE1	1:B:784:TYR:CE1	3.04	0.46
1:B:747:TYR:CZ	1:B:759:MET:HE2	2.51	0.46
1:B:805:ARG:CD	2:B:1115:HOH:O	2.61	0.46
1:B:651:VAL:HG21	1:B:804:LYS:HG2	1.97	0.46
1:B:801:GLN:OE1	1:B:801:GLN:HA	2.15	0.46
1:B:292:MET:O	1:B:294:GLU:N	2.48	0.46
1:A:17:THR:O	1:A:21:MET:HG3	2.16	0.46
1:A:519:TRP:O	1:A:522:GLU:HB2	2.15	0.46
1:B:637:ARG:NH1	2:B:1032:HOH:O	2.49	0.46
1:B:392:GLY:O	1:B:394:ALA:HB3	2.16	0.45
1:A:561:ARG:HB2	1:A:594:LEU:HD13	1.97	0.45
1:A:460:GLU:CD	1:A:460:GLU:H	2.24	0.45
1:A:528:ASN:O	1:A:529:PRO:C	2.59	0.45
1:B:592:ASP:O	1:B:595:MET:N	2.45	0.45
1:B:734:THR:HA	1:B:737:GLU:OE2	2.16	0.45
1:B:506:MET:SD	1:B:574:ARG:NE	2.90	0.45
1:B:593:ALA:O	1:B:596:ARG:HB3	2.17	0.45
1:A:723:TRP:CG	1:A:738:ARG:HH21	2.35	0.45
1:A:32:GLU:OE2	1:A:82:ARG:HD2	2.17	0.45
1:A:593:ALA:O	1:A:596:ARG:HB2	2.17	0.45
1:B:520:GLN:HA	1:B:523:VAL:HG13	1.99	0.45
1:B:224:ILE:HG23	1:B:371:THR:HG23	1.98	0.45
1:B:648:TYR:CZ	1:B:800:LYS:HB2	2.51	0.44
1:A:715:ASP:HB2	1:A:828:LYS:HG2	1.99	0.44
1:B:99:ILE:HD12	1:B:211:VAL:HG21	2.00	0.44
1:B:550:GLU:O	1:B:550:GLU:HG3	2.17	0.44
1:B:798:ASP:HA	1:B:799:PRO:HD2	1.75	0.44
1:A:503:ALA:CB	1:A:506:MET:HG2	2.47	0.44
1:A:370:GLN:OE1	1:A:776:LYS:HD3	2.17	0.44
1:A:503:ALA:HB1	1:A:506:MET:HG2	1.99	0.44
1:B:99:ILE:HB	1:B:409:THR:HB	1.99	0.44
1:B:223:LEU:HD11	1:B:377:PHE:CE1	2.53	0.44
1:A:594:LEU:HD21	1:A:597:ILE:HD11	2.00	0.44
1:B:230:GLU:OE2	1:B:368:GLU:O	2.34	0.44
1:A:228:PRO:HB3	1:A:367:ASN:HD21	1.82	0.43
1:A:504:THR:O	1:A:505:ASN:C	2.60	0.43
1:A:613:LYS:HA	1:A:614:PRO:HD2	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:GLN:HE22	1:B:800:LYS:NZ	2.15	0.43
1:B:718:LEU:O	1:B:719:PRO:C	2.60	0.43
1:B:789:ILE:O	1:B:789:ILE:CG2	2.65	0.43
1:B:782:MET:CE	1:B:810:MET:HE2	2.48	0.43
1:B:563:GLU:HG2	1:B:634:VAL:HG11	2.00	0.43
1:A:32:GLU:OE1	1:A:82:ARG:NH1	2.51	0.43
1:B:228:PRO:HB3	1:B:367:ASN:OD1	2.18	0.43
1:A:648:TYR:OH	1:A:800:LYS:N	2.51	0.43
1:B:679:ILE:HG13	1:B:823:ILE:HD11	2.01	0.43
1:B:14:ASN:HD21	1:B:411:VAL:H	1.67	0.43
1:A:701:TRP:CD1	1:A:701:TRP:N	2.85	0.43
1:A:82:ARG:O	1:A:83:HIS:C	2.62	0.43
1:B:594:LEU:C	1:B:596:ARG:N	2.76	0.43
1:B:283:GLU:O	1:B:287:VAL:HG12	2.19	0.42
1:B:514:VAL:O	2:B:957:HOH:O	2.21	0.42
1:B:703:ILE:O	1:B:706:LEU:N	2.49	0.42
1:A:440:GLU:O	1:A:444:GLU:HG2	2.19	0.42
1:A:620:HIS:HA	1:A:621:PRO:HD2	1.81	0.42
1:B:13:ARG:HD2	1:B:13:ARG:HA	1.84	0.42
1:B:103:ARG:CD	1:B:104:THR:H	2.32	0.42
1:B:392:GLY:C	1:B:394:ALA:N	2.78	0.42
1:A:773:SER:O	1:A:776:LYS:HG2	2.19	0.42
1:B:496:TYR:CG	1:B:497:PRO:HD2	2.54	0.42
1:A:666:LEU:HD22	1:A:672:VAL:HG21	2.00	0.42
1:B:16:ARG:HD3	1:B:16:ARG:HA	1.90	0.42
1:B:618:ILE:CA	2:B:1103:HOH:O	2.67	0.42
1:A:526:LEU:HD13	1:A:529:PRO:HA	2.01	0.42
1:A:799:PRO:O	1:A:800:LYS:O	2.30	0.42
1:B:285:LEU:HD23	1:B:310:VAL:HG21	2.02	0.42
1:B:542:GLN:HE21	1:B:546:ASP:CG	2.28	0.42
1:B:605:GLY:O	1:B:608:ARG:HG2	2.19	0.42
1:B:671:ASP:OD1	1:B:673:SER:OG	2.28	0.42
1:B:723:TRP:HB2	1:B:724:LEU:HD23	2.02	0.42
1:B:223:LEU:O	1:B:374:SER:HA	2.20	0.41
1:B:21:MET:HB2	1:B:21:MET:HE3	1.87	0.41
1:B:103:ARG:NH2	1:B:575:SER:O	2.53	0.41
1:B:198:ARG:HH21	1:B:664:ASN:HD22	1.67	0.41
1:B:788:GLY:C	1:B:792:ARG:HG3	2.44	0.41
1:A:365:ILE:HG22	1:A:366:GLN:O	2.20	0.41
1:A:412:VAL:HA	1:A:413:PRO:HD2	1.81	0.41
1:B:17:THR:HG22	1:B:21:MET:CE	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:GLY:O	1:B:394:ALA:CB	2.69	0.41
1:A:693:PRO:HA	1:A:694:PRO:HD3	1.92	0.41
1:A:727:GLU:HA	1:A:728:PRO:HD2	1.91	0.41
1:A:532:GLU:OE1	1:A:535:GLU:HB2	2.20	0.41
1:A:24:VAL:HG13	1:A:65:PRO:HG3	2.02	0.41
1:A:762:PHE:O	1:A:766:VAL:HG23	2.21	0.41
1:B:620:HIS:O	1:B:621:PRO:C	2.63	0.41
1:B:742:GLN:O	1:B:745:GLU:HG2	2.21	0.41
1:A:526:LEU:HD12	1:A:529:PRO:HB3	2.03	0.41
1:B:305:MET:HE1	1:B:784:TYR:HE2	1.86	0.41
1:B:706:LEU:C	1:B:706:LEU:CD1	2.93	0.41
1:B:782:MET:CE	1:B:810:MET:CE	2.99	0.41
1:B:396:THR:N	2:B:892:HOH:O	2.54	0.41
1:A:394:ALA:CA	2:A:980:HOH:O	2.44	0.40
1:B:557:ILE:HG23	1:B:587:TYR:CD2	2.57	0.40
1:B:510:GLY:HA3	1:B:574:ARG:HH12	1.87	0.40
1:B:441:ASP:HA	2:B:984:HOH:O	2.20	0.40
1:B:696:SER:HB3	1:B:700:MET:HB2	2.03	0.40
1:B:215:LEU:O	1:B:219:ALA:HB2	2.22	0.40

All (1) 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)
1:B:600:SER:OG	1:B:830:GLN:O[1_655]	1.97	0.23

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	682/853 (80%)	635 (93%)	31 (4%)	16 (2%)	5 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	717/853 (84%)	650 (91%)	39 (5%)	28 (4%)	2	1
All	All	1399/1706 (82%)	1285 (92%)	70 (5%)	44 (3%)	3	1

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	ALA
1	A	396	THR
1	A	507	ALA
1	A	599	ALA
1	A	614	PRO
1	A	730	LEU
1	B	229	ALA
1	B	293	ASP
1	B	302	ALA
1	B	394	ALA
1	B	395	ASP
1	B	599	ALA
1	B	612	MET
1	B	614	PRO
1	B	719	PRO
1	B	729	GLU
1	B	801	GLN
1	A	395	ASP
1	A	510	GLY
1	A	795	ALA
1	B	288	LYS
1	B	292	MET
1	B	393	THR
1	B	396	THR
1	B	510	GLY
1	B	597	ILE
1	B	619	GLU
1	B	704	PRO
1	A	603	VAL
1	A	619	GLU
1	B	289	GLU
1	B	368	GLU
1	B	796	GLN
1	B	797	LYS
1	A	800	LYS
1	A	801	GLN

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Mol	Chain	Res	Type
1	A	791	LEU
1	B	298	LEU
1	B	367	ASN
1	B	593	ALA
1	A	613	LYS
1	A	789	ILE
1	B	534	ILE
1	B	789	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	582/728 (80%)	525 (90%)	57 (10%)	7	5
1	B	613/728 (84%)	541 (88%)	72 (12%)	5	3
All	All	1195/1456 (82%)	1066 (89%)	129 (11%)	6	3

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	15	ASP
1	A	37	LYS
1	A	38	LEU
1	A	41	GLU
1	A	72	ARG
1	A	76	LYS
1	A	156	ILE
1	A	201	ARG
1	A	225	ILE
1	A	226	SER
1	A	365	ILE
1	A	366	GLN
1	A	369	ASN
1	A	393	THR

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Mol	Chain	Res	Type
1	A	395	ASP
1	A	406	LYS
1	A	409	THR
1	A	443	LYS
1	A	444	GLU
1	A	457	ILE
1	A	506	MET
1	A	509	ARG
1	A	518	SER
1	A	523	VAL
1	A	527	GLU
1	A	535	GLU
1	A	538	LYS
1	A	591	GLU
1	A	602	ARG
1	A	612	MET
1	A	613	LYS
1	A	614	PRO
1	A	618	ILE
1	A	632	ARG
1	A	635	GLU
1	A	636	SER
1	A	642	ARG
1	A	669	VAL
1	A	672	VAL
1	A	699	GLU
1	A	708	GLU
1	A	711	LYS
1	A	725	ASP
1	A	730	LEU
1	A	731	HIS
1	A	734	THR
1	A	735	LEU
1	A	738	ARG
1	A	742	GLN
1	A	754	VAL
1	A	789	ILE
1	A	791	LEU
1	A	792	ARG
1	A	797	LYS
1	A	800	LYS
1	A	816	GLU

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Mol	Chain	Res	Type
1	B	12	SER
1	B	16	ARG
1	B	37	LYS
1	B	38	LEU
1	B	103	ARG
1	B	156	ILE
1	B	196	GLU
1	B	226	SER
1	B	230	GLU
1	B	231	ASP
1	B	282	ILE
1	B	283	GLU
1	B	285	LEU
1	B	286	LEU
1	B	288	LYS
1	B	291	ILE
1	B	293	ASP
1	B	299	TYR
1	B	306	LEU
1	B	310	VAL
1	B	367	ASN
1	B	368	GLU
1	B	393	THR
1	B	409	THR
1	B	431	GLU
1	B	457	ILE
1	B	459	ILE
1	B	461	LYS
1	B	506	MET
1	B	512	ASP
1	B	520	GLN
1	B	523	VAL
1	B	526	LEU
1	B	527	GLU
1	B	532	GLU
1	B	535	GLU
1	B	589	SER
1	B	594	LEU
1	B	595	MET
1	B	596	ARG
1	B	602	ARG
1	B	604	SER

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Mol	Chain	Res	Type
1	B	609	LYS
1	B	610	LEU
1	B	612	MET
1	B	625	LYS
1	B	637	ARG
1	B	657	ARG
1	B	670	SER
1	B	672	VAL
1	B	679	ILE
1	B	696	SER
1	B	703	ILE
1	B	706	LEU
1	B	707	GLN
1	B	718	LEU
1	B	722	GLU
1	B	724	LEU
1	B	725	ASP
1	B	726	LYS
1	B	727	GLU
1	B	734	THR
1	B	742	GLN
1	B	779	LEU
1	B	783	ASP
1	B	791	LEU
1	B	796	GLN
1	B	800	LYS
1	B	801	GLN
1	B	821	GLU
1	B	831	VAL
1	B	832	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	486	ASN
1	A	520	GLN
1	A	533	GLN
1	A	562	HIS
1	A	570	GLN
1	A	638	ASN
1	A	662	GLN

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Mol	Chain	Res	Type
1	A	742	GLN
1	A	748	GLN
1	A	790	HIS
1	B	14	ASN
1	B	467	ASN
1	B	520	GLN
1	B	528	ASN
1	B	533	GLN
1	B	542	GLN
1	B	545	HIS
1	B	620	HIS
1	B	629	ASN
1	B	638	ASN
1	B	644	GLN
1	B	664	ASN
1	B	707	GLN
1	B	761	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 ⓘ

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	686/853 (80%)	1.52	171 (24%) 2 1	40, 53, 84, 102	0
1	B	723/853 (84%)	1.97	276 (38%) 1 1	38, 54, 87, 102	0
All	All	1409/1706 (82%)	1.75	447 (31%) 1 1	38, 53, 86, 102	0

All (447) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	728	PRO	10.7
1	A	597	ILE	10.5
1	B	789	ILE	8.9
1	B	598	PHE	8.7
1	B	291	ILE	8.3
1	B	603	VAL	8.2
1	B	615	GLY	8.2
1	B	283	GLU	8.0
1	B	597	ILE	7.9
1	B	365	ILE	7.7
1	A	603	VAL	6.9
1	A	791	LEU	6.9
1	B	299	TYR	6.8
1	B	697	LEU	6.8
1	B	700	MET	6.7
1	A	394	ALA	6.6
1	B	721	ALA	6.6
1	B	724	LEU	6.5
1	B	723	TRP	6.3
1	B	696	SER	6.3
1	B	614	PRO	6.2
1	B	12	SER	6.1
1	B	718	LEU	6.1
1	A	794	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	282	ILE	6.0
1	B	393	THR	6.0
1	B	610	LEU	6.0
1	B	703	ILE	6.0
1	B	735	LEU	5.9
1	B	791	LEU	5.8
1	A	723	TRP	5.8
1	B	507	ALA	5.8
1	A	507	ALA	5.7
1	B	594	LEU	5.7
1	B	730	LEU	5.7
1	A	616	GLU	5.7
1	B	795	ALA	5.7
1	B	684	PHE	5.5
1	B	292	MET	5.4
1	B	394	ALA	5.4
1	B	731	HIS	5.4
1	A	604	SER	5.4
1	A	614	PRO	5.3
1	B	691	TYR	5.3
1	A	365	ILE	5.3
1	B	287	VAL	5.3
1	B	796	GLN	5.3
1	B	704	PRO	5.2
1	B	706	LEU	5.2
1	B	794	TYR	5.2
1	B	229	ALA	5.2
1	B	695	GLN	5.1
1	A	724	LEU	5.1
1	B	280	VAL	5.1
1	B	607	MET	5.1
1	A	594	LEU	5.1
1	B	734	THR	5.1
1	A	720	ILE	5.0
1	A	728	PRO	5.0
1	B	483	PHE	5.0
1	B	725	ASP	4.9
1	B	705	GLY	4.9
1	A	610	LEU	4.9
1	A	395	ASP	4.9
1	A	617	ALA	4.8
1	B	521	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	616	GLU	4.8
1	A	602	ARG	4.8
1	A	612	MET	4.8
1	A	534	ILE	4.7
1	A	799	PRO	4.7
1	B	609	LYS	4.7
1	B	702	ASP	4.7
1	A	796	GLN	4.7
1	B	509	ARG	4.7
1	B	602	ARG	4.7
1	A	598	PHE	4.6
1	B	790	HIS	4.6
1	A	725	ASP	4.6
1	B	285	LEU	4.6
1	A	792	ARG	4.6
1	A	721	ALA	4.6
1	B	719	PRO	4.6
1	B	290	GLY	4.5
1	B	793	GLY	4.5
1	B	281	LEU	4.5
1	A	797	LYS	4.5
1	A	615	GLY	4.5
1	B	618	ILE	4.5
1	A	531	ALA	4.5
1	A	705	GLY	4.4
1	A	793	GLY	4.4
1	A	15	ASP	4.4
1	B	688	ILE	4.4
1	B	617	ALA	4.4
1	B	831	VAL	4.4
1	A	716	LEU	4.4
1	B	720	ILE	4.4
1	B	611	GLY	4.3
1	A	717	ASP	4.3
1	A	727	GLU	4.3
1	A	789	ILE	4.3
1	B	301	PRO	4.3
1	A	593	ALA	4.3
1	B	729	GLU	4.3
1	B	599	ALA	4.3
1	B	738	ARG	4.3
1	B	230	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	699	GLU	4.2
1	B	727	GLU	4.2
1	A	16	ARG	4.2
1	B	103	ARG	4.2
1	A	731	HIS	4.2
1	A	600	SER	4.2
1	B	832	ARG	4.2
1	A	715	ASP	4.1
1	B	694	PRO	4.1
1	B	797	LYS	4.1
1	B	593	ALA	4.1
1	B	284	GLU	4.1
1	B	670	SER	4.1
1	B	286	LEU	4.0
1	B	367	ASN	4.0
1	B	519	TRP	4.0
1	A	523	VAL	4.0
1	B	595	MET	4.0
1	B	792	ARG	4.0
1	A	722	GLU	4.0
1	B	606	MET	4.0
1	B	709	ARG	4.0
1	A	834	PRO	3.9
1	B	740	LEU	3.9
1	A	14	ASN	3.9
1	B	513	ILE	3.9
1	B	692	ILE	3.9
1	A	718	LEU	3.9
1	B	701	TRP	3.8
1	B	605	GLY	3.8
1	A	367	ASN	3.8
1	B	524	ALA	3.8
1	A	719	PRO	3.8
1	A	618	ILE	3.8
1	A	368	GLU	3.8
1	B	689	ASP	3.7
1	B	508	GLY	3.7
1	B	506	MET	3.7
1	B	739	ILE	3.7
1	B	313	ALA	3.7
1	A	709	ARG	3.7
1	A	700	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	599	ALA	3.7
1	B	395	ASP	3.7
1	A	17	THR	3.7
1	A	396	THR	3.7
1	B	136	ALA	3.7
1	A	784	TYR	3.7
1	A	790	HIS	3.6
1	B	604	SER	3.6
1	B	714	PHE	3.6
1	B	612	MET	3.6
1	A	526	LEU	3.6
1	A	798	ASP	3.6
1	B	596	ARG	3.6
1	B	600	SER	3.6
1	A	393	THR	3.5
1	B	532	GLU	3.5
1	B	608	ARG	3.5
1	A	613	LYS	3.5
1	B	228	PRO	3.5
1	B	708	GLU	3.5
1	B	722	GLU	3.5
1	B	754	VAL	3.5
1	A	398	ALA	3.5
1	A	697	LEU	3.5
1	A	607	MET	3.5
1	B	429	MET	3.5
1	B	669	VAL	3.5
1	B	15	ASP	3.4
1	B	733	GLU	3.4
1	B	366	GLN	3.4
1	A	833	MET	3.4
1	A	609	LYS	3.4
1	A	745	GLU	3.4
1	B	295	GLY	3.4
1	A	795	ALA	3.4
1	B	510	GLY	3.3
1	A	601	ASP	3.3
1	B	687	THR	3.3
1	A	704	PRO	3.3
1	B	526	LEU	3.3
1	A	691	TYR	3.3
1	B	820	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	302	ALA	3.3
1	B	296	GLU	3.3
1	B	613	LYS	3.2
1	A	595	MET	3.2
1	B	534	ILE	3.2
1	B	716	LEU	3.2
1	A	831	VAL	3.2
1	B	753	VAL	3.2
1	B	693	PRO	3.2
1	A	726	LYS	3.2
1	B	293	ASP	3.1
1	B	479	LEU	3.1
1	B	232	SER	3.1
1	A	832	ARG	3.1
1	A	806	GLU	3.1
1	B	472	ALA	3.1
1	B	717	ASP	3.1
1	B	523	VAL	3.1
1	B	746	VAL	3.1
1	A	508	GLY	3.0
1	B	303	ASN	3.0
1	B	530	THR	3.0
1	A	708	GLU	3.0
1	B	752	GLU	3.0
1	B	711	LYS	3.0
1	B	742	GLN	3.0
1	A	687	THR	3.0
1	A	519	TRP	3.0
1	B	743	SER	3.0
1	A	698	GLU	3.0
1	B	531	ALA	2.9
1	A	730	LEU	2.9
1	B	710	LEU	2.9
1	B	126	VAL	2.9
1	A	710	LEU	2.9
1	A	672	VAL	2.9
1	A	216	ILE	2.9
1	B	713	ASP	2.9
1	B	799	PRO	2.9
1	B	368	GLU	2.9
1	A	735	LEU	2.9
1	B	511	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	294	GLU	2.9
1	B	122	THR	2.8
1	B	641	ILE	2.8
1	B	732	GLU	2.8
1	B	747	TYR	2.8
1	A	606	MET	2.8
1	B	156	ILE	2.8
1	B	297	SER	2.8
1	A	742	GLN	2.8
1	A	611	GLY	2.8
1	A	30	ALA	2.8
1	B	686	ALA	2.8
1	A	193	PHE	2.8
1	B	690	ALA	2.8
1	B	288	LYS	2.8
1	B	308	HIS	2.7
1	A	209	ASP	2.7
1	A	757	GLU	2.7
1	B	488	ALA	2.7
1	A	530	THR	2.7
1	A	366	GLN	2.7
1	B	129	VAL	2.7
1	B	310	VAL	2.7
1	B	707	GLN	2.7
1	B	829	VAL	2.7
1	B	170	TYR	2.7
1	B	788	GLY	2.7
1	B	749	ARG	2.7
1	A	481	ALA	2.7
1	A	512	ASP	2.7
1	A	19	ARG	2.7
1	A	596	ARG	2.6
1	B	745	GLU	2.6
1	A	539	ALA	2.6
1	A	228	PRO	2.6
1	B	94	LEU	2.6
1	A	103	ARG	2.6
1	A	560	GLU	2.6
1	B	312	ALA	2.6
1	B	203	LEU	2.6
1	B	214	ILE	2.6
1	A	13	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	488	ALA	2.6
1	B	16	ARG	2.6
1	B	407	LEU	2.6
1	A	639	PHE	2.5
1	B	737	GLU	2.5
1	A	744	ILE	2.5
1	B	27	ILE	2.5
1	A	369	ASN	2.5
1	A	511	THR	2.5
1	B	396	THR	2.5
1	B	409	THR	2.5
1	B	159	PRO	2.5
1	B	93	VAL	2.5
1	B	154	VAL	2.5
1	B	512	ASP	2.5
1	B	481	ALA	2.5
1	B	158	LEU	2.5
1	A	684	PHE	2.5
1	B	125	GLY	2.5
1	A	537	ILE	2.5
1	B	174	ILE	2.5
1	A	712	ASN	2.5
1	B	528	ASN	2.5
1	B	712	ASN	2.5
1	A	690	ALA	2.5
1	B	206	ALA	2.5
1	A	399	PHE	2.5
1	A	608	ARG	2.5
1	B	13	ARG	2.5
1	B	736	ARG	2.5
1	A	669	VAL	2.4
1	A	754	VAL	2.4
1	B	491	VAL	2.4
1	B	822	VAL	2.4
1	A	810	MET	2.4
1	B	489	ALA	2.4
1	A	711	LYS	2.4
1	B	726	LYS	2.4
1	A	509	ARG	2.4
1	B	632	ARG	2.4
1	B	486	ASN	2.4
1	B	304	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	698	GLU	2.4
1	B	211	VAL	2.4
1	B	715	ASP	2.4
1	B	202	LYS	2.4
1	B	298	LEU	2.4
1	A	714	PHE	2.4
1	A	702	ASP	2.4
1	B	71	VAL	2.4
1	B	744	ILE	2.4
1	A	506	MET	2.4
1	B	482	LYS	2.4
1	A	433	GLU	2.4
1	A	409	THR	2.4
1	B	311	THR	2.4
1	B	806	GLU	2.3
1	A	483	PHE	2.3
1	A	567	ILE	2.3
1	B	487	GLU	2.3
1	B	520	GLN	2.3
1	B	176	TYR	2.3
1	B	492	ALA	2.3
1	A	135	LEU	2.3
1	B	123	GLY	2.3
1	B	231	ASP	2.3
1	A	688	ILE	2.3
1	A	522	GLU	2.3
1	A	635	GLU	2.3
1	B	514	VAL	2.3
1	B	186	TYR	2.3
1	A	637	ARG	2.3
1	A	800	LYS	2.3
1	A	429	MET	2.3
1	A	641	ILE	2.3
1	B	567	ILE	2.3
1	B	59	VAL	2.3
1	B	128	VAL	2.3
1	B	410	VAL	2.3
1	B	798	ASP	2.3
1	B	60	LEU	2.3
1	B	571	LEU	2.3
1	A	533	GLN	2.2
1	B	399	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	749	ARG	2.2
1	A	406	LYS	2.2
1	A	682	ASP	2.2
1	A	787	GLN	2.2
1	B	402	SER	2.2
1	A	734	THR	2.2
1	A	418	MET	2.2
1	B	307	MET	2.2
1	B	755	GLY	2.2
1	A	686	ALA	2.2
1	B	116	ALA	2.2
1	B	172	ALA	2.2
1	B	652	ALA	2.2
1	B	150	LEU	2.2
1	B	207	LEU	2.2
1	A	620	HIS	2.2
1	B	182	TYR	2.2
1	B	205	TYR	2.2
1	B	99	ILE	2.2
1	B	419	ILE	2.2
1	A	527	GLU	2.2
1	B	107	GLY	2.2
1	A	741	ALA	2.2
1	B	636	SER	2.2
1	B	678	SER	2.2
1	B	786	ARG	2.2
1	A	621	PRO	2.1
1	B	104	THR	2.2
1	B	529	PRO	2.1
1	A	732	GLU	2.1
1	B	289	GLU	2.1
1	B	543	VAL	2.1
1	B	525	ALA	2.1
1	B	110	LEU	2.1
1	A	149	PHE	2.1
1	A	692	ILE	2.1
1	B	679	ILE	2.1
1	A	746	VAL	2.1
1	B	309	HIS	2.1
1	A	20	ARG	2.1
1	B	637	ARG	2.1
1	B	67	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	56	LYS	2.1
1	A	571	LEU	2.1
1	B	118	LEU	2.1
1	B	518	SER	2.1
1	A	563	GLU	2.1
1	B	408	ASP	2.1
1	A	830	GLN	2.1
1	A	642	ARG	2.1
1	B	404	ILE	2.1
1	B	457	ILE	2.1
1	B	37	LYS	2.1
1	B	590	MET	2.1
1	B	505	ASN	2.1
1	A	689	ASP	2.1
1	A	707	GLN	2.1
1	A	685	LYS	2.1
1	A	184	PHE	2.1
1	A	535	GLU	2.0
1	A	652	ALA	2.1
1	B	100	ALA	2.1
1	B	305	MET	2.0
1	B	601	ASP	2.0
1	B	682	ASP	2.0
1	B	17	THR	2.0
1	B	153	THR	2.0
1	B	124	LYS	2.0
1	B	685	LYS	2.0
1	A	227	GLY	2.0
1	A	703	ILE	2.0
1	B	537	ILE	2.0
1	A	729	GLU	2.0
1	B	184	PHE	2.0
1	B	377	PHE	2.0
1	B	672	VAL	2.0
1	B	751	GLU	2.0
1	B	757	GLU	2.0
1	A	521	ALA	2.0
1	B	388	ALA	2.0
1	B	369	ASN	2.0
1	B	54	LEU	2.0
1	B	121	LEU	2.0
1	B	383	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	625	LYS	2.0
1	A	788	GLY	2.0
1	A	820	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.