



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 04:49 PM EDT

PDB ID : 3DL8 / pdb_00003dl8
Title : Structure of the complex of aquifex aeolicus SecYEG and bacillus subtilis SecA
Authors : Nam, Y.; Zimmer, J.; Rapoport, T.A.
Deposited on : 2008-06-26
Resolution : 7.50 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

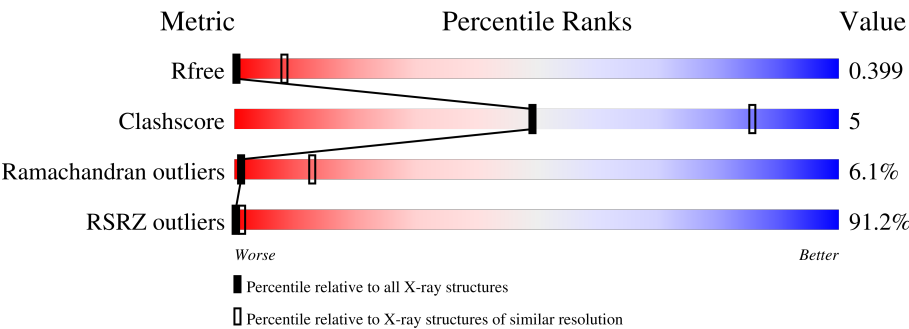
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.50 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	779	92% 85% 14%
1	B	779	93% 86% 13%
2	G	429	84% 78% 14% 5%
2	H	429	85% 79% 14% 5%
3	C	65	51% 52% 46%
3	D	65	48% 52% 46%
4	E	107	49% 54% 7% 39%

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Mol	Chain	Length	Quality of chain
4	F	107	48% 54% 7% 39%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10232 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 Protein translocase subunit secA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	0	0	0
			3092	1546	773	773			
1	B	773	Total	C	N	O	0	0	0
			3092	1546	773	773			

- Molecule 2 is a protein called Preprotein translocase subunit secY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	406	Total	C	N	O	0	0	0
			1624	812	406	406			
2	H	406	Total	C	N	O	0	0	0
			1624	812	406	406			

- Molecule 3 is a protein called SecE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	35	Total	C	N	O	0	0	0
			140	70	35	35			
3	D	35	Total	C	N	O	0	0	0
			140	70	35	35			

- Molecule 4 is a protein called Protein-export membrane protein secG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	65	Total	C	N	O	0	0	0
			260	130	65	65			
4	F	65	Total	C	N	O	0	0	0
			260	130	65	65			

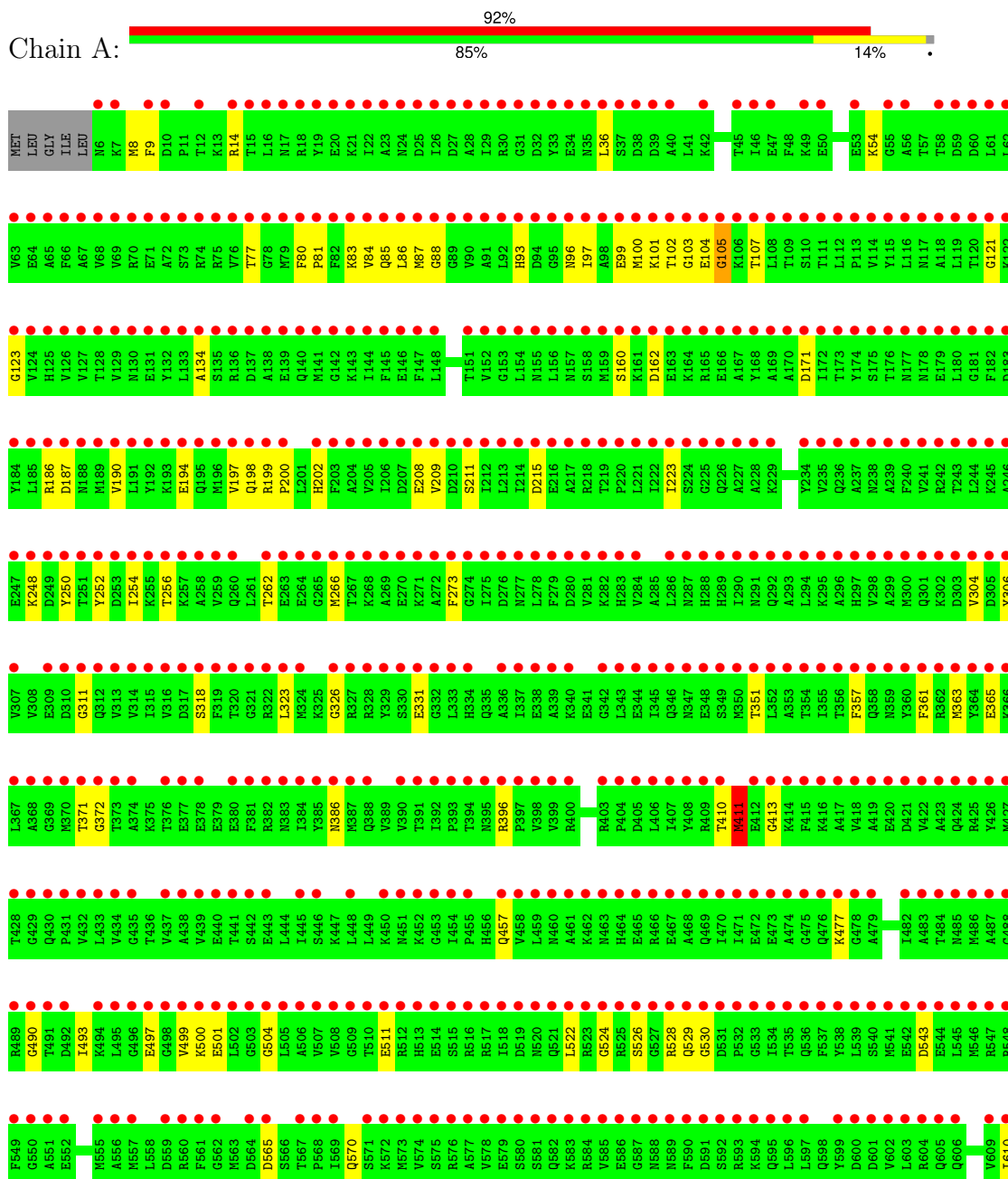
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	101	GLY	-	expression tag	UNP O66505
E	102	HIS	-	expression tag	UNP O66505
E	103	HIS	-	insertion	UNP O66505
E	104	HIS	-	expression tag	UNP O66505
E	105	HIS	-	expression tag	UNP O66505
E	106	HIS	-	expression tag	UNP O66505
E	107	HIS	-	expression tag	UNP O66505
F	101	GLY	-	expression tag	UNP O66505
F	102	HIS	-	expression tag	UNP O66505
F	103	HIS	-	expression tag	UNP O66505
F	104	HIS	-	expression tag	UNP O66505
F	105	HIS	-	expression tag	UNP O66505
F	106	HIS	-	expression tag	UNP O66505
F	107	HIS	-	expression tag	UNP O66505

3 Residue-property plots

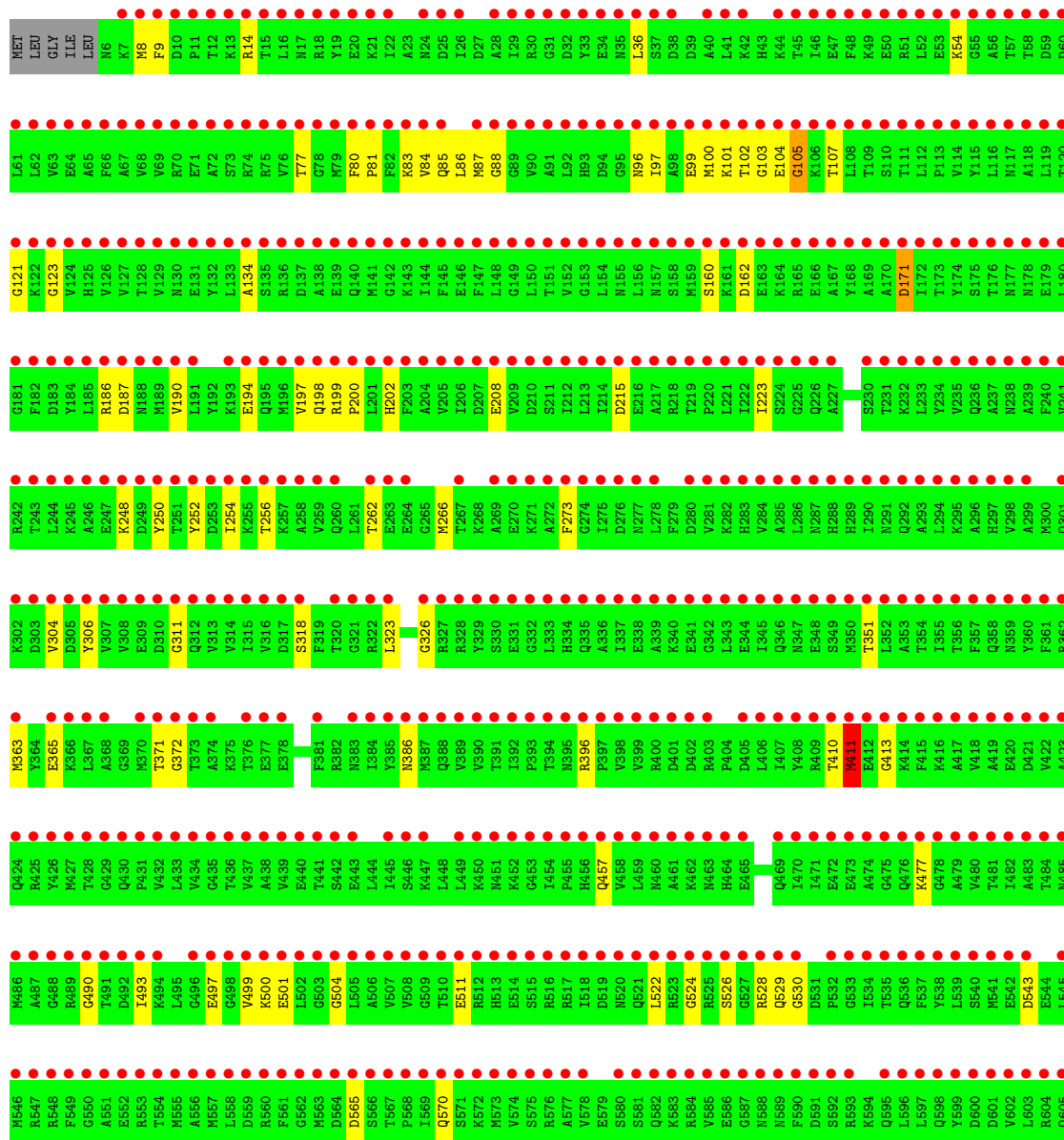
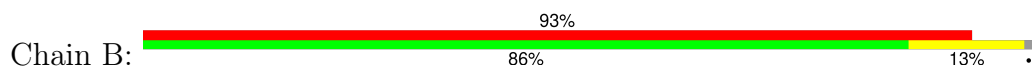
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



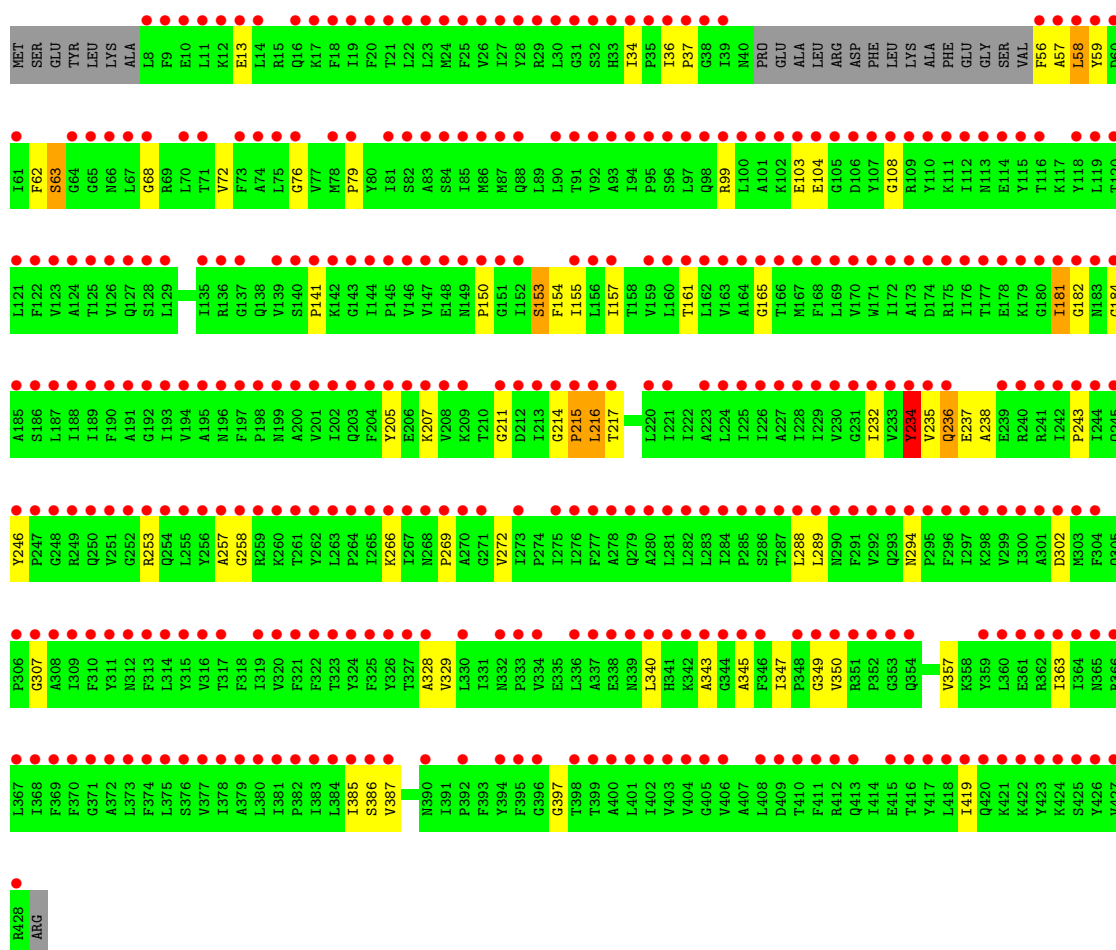
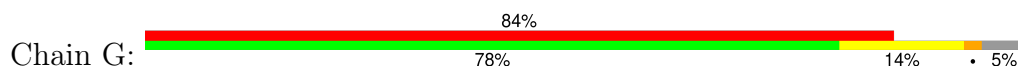


• Molecule 1: Protein translocase subunit secA

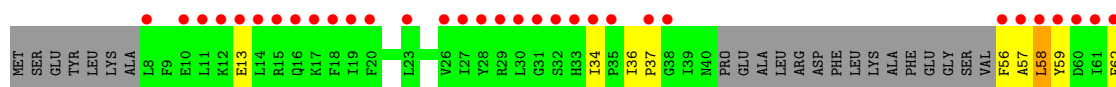
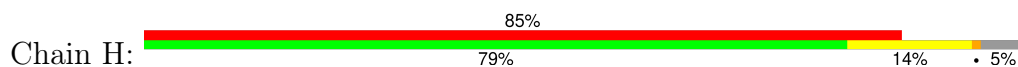


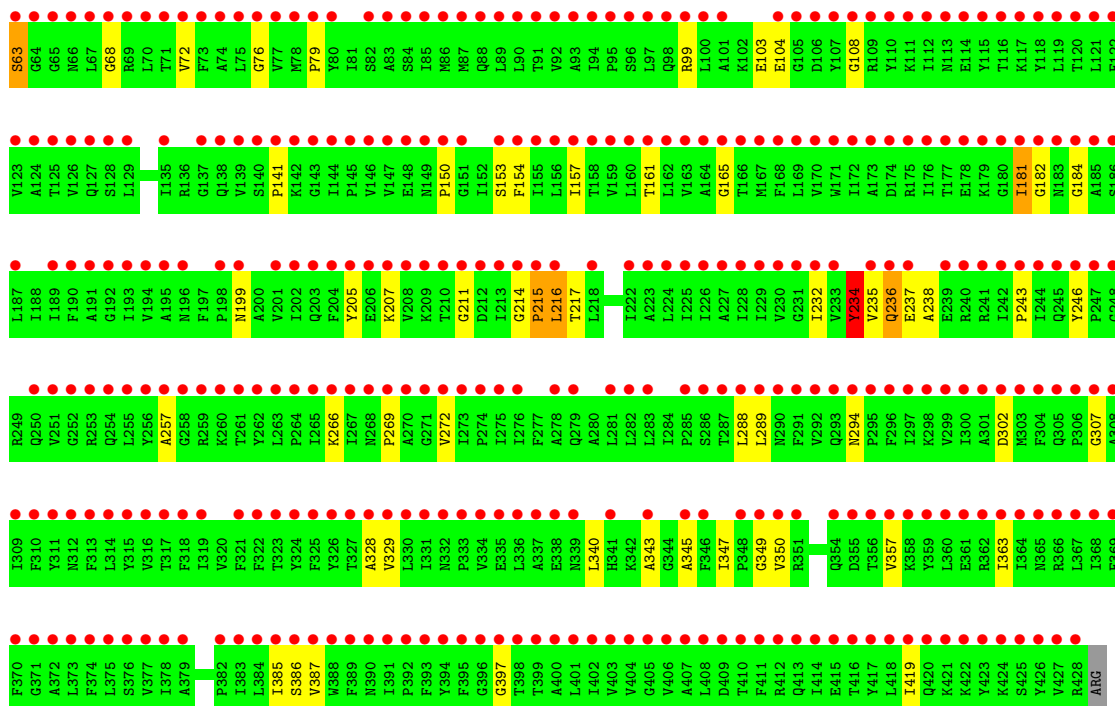


• Molecule 2: Preprotein translocase subunit secY

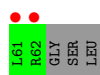
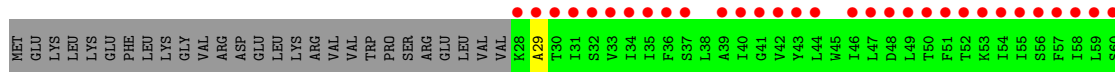


• Molecule 2: Preprotein translocase subunit secY

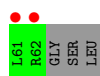
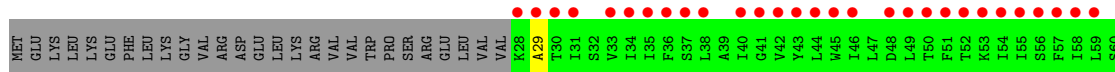




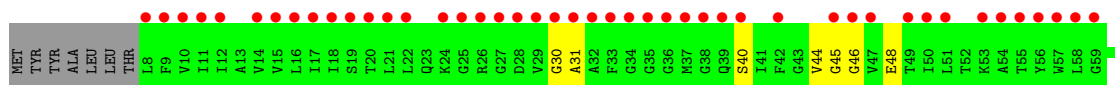
- Molecule 3: SecE

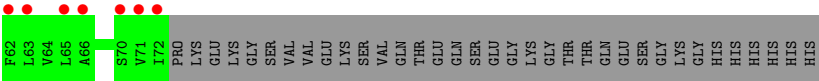


- Molecule 3: SecE

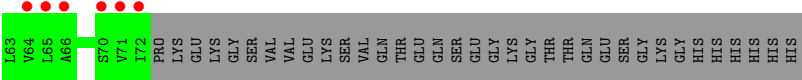
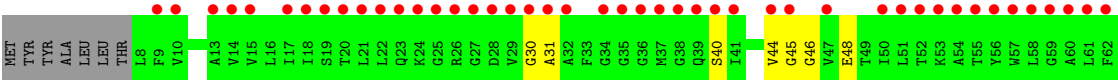


- Molecule 4: Protein-export membrane protein secY





● Molecule 4: Protein-export membrane protein secG



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	146.36Å 167.97Å 187.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 7.50 14.99 – 7.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (14.99-7.50) 86.0 (14.99-7.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 7.37Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.365 , 0.390 0.397 , 0.399	Depositor DCC
R_{free} test set	604 reflections (9.72%)	wwPDB-VP
Wilson B-factor (Å ²)	530.1	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.34 , 359.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	10232	wwPDB-VP
Average B, all atoms (Å ²)	452.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% 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	1.52	1/3091 (0.0%)	1.73	50/3862 (1.3%)
1	B	1.52	1/3091 (0.0%)	1.73	51/3862 (1.3%)
2	G	1.68	4/1622 (0.2%)	1.79	31/2024 (1.5%)
2	H	1.68	4/1622 (0.2%)	1.79	32/2024 (1.6%)
3	C	1.66	0/139	1.56	1/172 (0.6%)
3	D	1.67	0/139	1.56	1/172 (0.6%)
4	E	1.66	0/259	1.73	5/322 (1.6%)
4	F	1.65	0/259	1.72	5/322 (1.6%)
All	All	1.58	10/10222 (0.1%)	1.75	176/12760 (1.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	181	ILE	CA-C	-7.64	1.43	1.52
2	G	181	ILE	CA-C	-7.63	1.43	1.52
1	B	653	LYS	CA-C	-5.78	1.49	1.52
1	A	653	LYS	CA-C	-5.68	1.49	1.52
2	G	294	ASN	CA-C	-5.63	1.49	1.53
2	H	234	TYR	CA-C	-5.63	1.45	1.52
2	H	294	ASN	CA-C	-5.59	1.49	1.53
2	G	234	TYR	CA-C	-5.53	1.45	1.52
2	G	182	GLY	N-CA	-5.14	1.39	1.45
2	H	182	GLY	N-CA	-5.11	1.39	1.45

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	SER	N-CA-C	-10.93	91.59	109.40
1	B	160	SER	N-CA-C	-10.90	91.63	109.40
2	G	154	PHE	N-CA-C	-10.63	99.57	112.54
2	H	154	PHE	N-CA-C	-10.62	99.58	112.54
4	F	45	GLY	N-CA-C	-10.06	101.17	114.25
4	E	45	GLY	N-CA-C	-10.02	101.23	114.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	VAL	CA-C-N	8.89	137.41	122.65
1	A	304	VAL	C-N-CA	8.89	137.41	122.65
1	B	304	VAL	CA-C-N	8.83	137.31	122.65
1	B	304	VAL	C-N-CA	8.83	137.31	122.65
2	H	302	ASP	CA-C-N	-8.81	108.31	122.66
2	H	302	ASP	C-N-CA	-8.81	108.31	122.66
2	G	302	ASP	CA-C-N	-8.70	108.49	122.66
2	G	302	ASP	C-N-CA	-8.70	108.49	122.66
1	A	87	MET	N-CA-C	-7.99	102.52	111.71
1	B	87	MET	N-CA-C	-7.99	102.52	111.71
2	H	182	GLY	N-CA-C	-7.99	103.14	112.73
2	G	182	GLY	N-CA-C	-7.91	103.24	112.73
1	A	639	ILE	CA-C-N	7.58	133.57	120.68
1	A	639	ILE	C-N-CA	7.58	133.57	120.68
1	A	223	ILE	N-CA-C	7.54	118.57	111.48
1	B	639	ILE	CA-C-N	7.51	133.45	120.68
1	B	639	ILE	C-N-CA	7.51	133.45	120.68
1	B	223	ILE	N-CA-C	7.47	118.51	111.48
1	B	208	GLU	CA-C-N	7.24	131.91	120.47
1	B	208	GLU	C-N-CA	7.24	131.91	120.47
1	A	208	GLU	CA-C-N	7.21	131.87	120.47
1	A	208	GLU	C-N-CA	7.21	131.87	120.47
1	B	9	PHE	N-CA-C	-7.17	103.50	111.82
2	H	211	GLY	N-CA-C	-7.12	105.39	115.43
1	A	311	GLY	N-CA-C	-7.08	103.97	113.24
2	G	211	GLY	N-CA-C	-7.07	105.45	115.43
1	A	9	PHE	N-CA-C	-7.06	103.59	111.71
1	B	311	GLY	N-CA-C	-7.04	104.01	113.24
2	H	216	LEU	N-CA-C	-7.04	103.61	111.71
2	G	235	VAL	CA-C-N	7.03	134.97	121.54
2	G	235	VAL	C-N-CA	7.03	134.97	121.54
2	H	235	VAL	CA-C-N	6.97	134.85	121.54
2	H	235	VAL	C-N-CA	6.97	134.85	121.54
2	G	216	LEU	N-CA-C	-6.94	103.73	111.71
1	B	250	TYR	CA-C-N	6.91	133.87	121.92
1	B	250	TYR	C-N-CA	6.91	133.87	121.92
1	A	250	TYR	CA-C-N	6.89	133.85	121.92
1	A	250	TYR	C-N-CA	6.89	133.85	121.92
2	G	238	ALA	N-CA-C	6.87	117.66	108.38
2	H	238	ALA	N-CA-C	6.86	117.64	108.38
1	B	83	LYS	N-CA-C	6.70	121.69	112.04
1	A	83	LYS	N-CA-C	6.64	121.61	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	MET	N-CA-C	-6.62	104.06	111.28
1	A	363	MET	N-CA-C	-6.56	104.12	111.28
4	F	31	ALA	CA-C-N	6.51	131.02	120.60
4	F	31	ALA	C-N-CA	6.51	131.02	120.60
4	E	31	ALA	CA-C-N	6.43	130.90	120.60
4	E	31	ALA	C-N-CA	6.43	130.90	120.60
1	A	646	GLU	N-CA-C	-6.38	104.32	111.28
1	B	372	GLY	CA-C-N	6.33	132.98	122.54
1	B	372	GLY	C-N-CA	6.33	132.98	122.54
2	G	72	VAL	N-CA-C	-6.31	104.18	110.62
2	G	266	LYS	N-CA-C	6.31	121.01	113.12
2	H	266	LYS	N-CA-C	6.31	121.01	113.12
1	A	199	ARG	N-CA-C	-6.29	101.05	110.24
2	H	72	VAL	N-CA-C	-6.26	104.23	110.62
1	A	372	GLY	CA-C-N	6.25	132.86	122.54
1	A	372	GLY	C-N-CA	6.25	132.86	122.54
1	B	199	ARG	N-CA-C	-6.24	101.13	110.24
1	B	646	GLU	N-CA-C	-6.22	104.50	111.28
1	B	194	GLU	N-CA-C	-6.20	104.58	111.71
1	A	248	LYS	CA-C-N	6.17	128.55	120.28
1	A	248	LYS	C-N-CA	6.17	128.55	120.28
1	A	194	GLU	N-CA-C	-6.13	104.66	111.71
1	B	248	LYS	CA-C-N	6.08	128.43	120.28
1	B	248	LYS	C-N-CA	6.08	128.43	120.28
1	A	186	ARG	CA-C-N	6.05	133.10	121.54
1	A	186	ARG	C-N-CA	6.05	133.10	121.54
1	B	186	ARG	CA-C-N	6.02	133.04	121.54
1	B	186	ARG	C-N-CA	6.02	133.04	121.54
2	G	307	GLY	N-CA-C	-5.98	108.09	114.67
2	H	307	GLY	N-CA-C	-5.95	108.12	114.67
1	A	411	MET	CA-C-N	5.91	132.84	121.54
1	A	411	MET	C-N-CA	5.91	132.84	121.54
1	B	411	MET	CA-C-N	5.90	132.81	121.54
1	B	411	MET	C-N-CA	5.90	132.81	121.54
2	G	215	PRO	N-CA-C	-5.90	107.12	114.20
2	H	215	PRO	N-CA-C	-5.88	107.15	114.20
1	A	84	VAL	CA-C-N	5.86	130.50	120.71
1	A	84	VAL	C-N-CA	5.86	130.50	120.71
1	B	202	HIS	N-CA-C	5.86	120.22	111.96
1	A	202	HIS	N-CA-C	5.84	120.20	111.96
1	B	637	ARG	N-CA-C	-5.84	104.99	111.71
2	G	363	ILE	CA-C-N	-5.83	113.10	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	363	ILE	C-N-CA	-5.83	113.10	120.56
1	B	84	VAL	CA-C-N	5.82	130.44	120.71
1	B	84	VAL	C-N-CA	5.82	130.44	120.71
2	H	363	ILE	CA-C-N	-5.80	113.14	120.56
2	H	363	ILE	C-N-CA	-5.80	113.14	120.56
2	H	246	TYR	N-CA-C	-5.79	102.30	110.29
1	A	637	ARG	N-CA-C	-5.78	105.06	111.71
2	H	104	GLU	N-CA-C	-5.76	103.99	113.50
2	G	246	TYR	N-CA-C	-5.76	102.34	110.29
1	A	457	GLN	CA-C-N	-5.76	115.41	123.13
1	A	457	GLN	C-N-CA	-5.76	115.41	123.13
2	H	79	PRO	N-CA-C	-5.75	106.67	113.86
1	B	54	LYS	CA-C-N	5.75	132.67	121.41
1	B	54	LYS	C-N-CA	5.75	132.67	121.41
1	A	54	LYS	CA-C-N	5.74	132.67	121.41
1	A	54	LYS	C-N-CA	5.74	132.67	121.41
1	B	522	LEU	N-CA-C	-5.72	105.04	111.28
2	G	104	GLU	N-CA-C	-5.68	104.12	113.50
1	A	522	LEU	N-CA-C	-5.66	105.11	111.28
1	B	610	ILE	N-CA-C	5.63	115.77	110.30
2	G	79	PRO	N-CA-C	-5.62	106.84	113.86
1	B	457	GLN	CA-C-N	-5.58	115.65	123.13
1	B	457	GLN	C-N-CA	-5.58	115.65	123.13
2	G	184	GLY	N-CA-C	-5.54	105.68	112.77
2	H	184	GLY	N-CA-C	-5.54	105.69	112.77
2	H	288	LEU	N-CA-C	-5.46	105.33	111.28
1	B	160	SER	CA-C-O	-5.45	114.81	120.70
1	A	14	ARG	N-CA-C	-5.45	105.34	111.28
1	A	610	ILE	N-CA-C	5.43	115.57	110.30
4	E	48	GLU	N-CA-C	-5.42	101.88	109.69
1	B	14	ARG	N-CA-C	-5.42	105.37	111.28
4	F	48	GLU	N-CA-C	-5.39	101.93	109.69
2	H	357	VAL	N-CA-C	-5.37	104.34	111.05
2	G	288	LEU	N-CA-C	-5.36	105.44	111.28
2	G	357	VAL	N-CA-C	-5.32	104.41	111.05
1	A	81	PRO	N-CA-C	5.31	123.41	112.47
2	G	238	ALA	CA-C-N	5.31	131.68	121.54
2	G	238	ALA	C-N-CA	5.31	131.68	121.54
1	A	160	SER	CA-C-O	-5.30	114.97	120.70
1	A	754	MET	N-CA-C	-5.30	104.75	111.11
1	B	121	GLY	N-CA-C	-5.30	107.79	115.27
2	H	238	ALA	CA-C-N	5.30	131.67	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	238	ALA	C-N-CA	5.30	131.67	121.54
1	B	623	LEU	N-CA-C	-5.30	106.77	113.18
1	A	699	LYS	N-CA-C	-5.29	105.52	111.28
1	B	754	MET	N-CA-C	-5.29	104.77	111.11
3	C	29	ALA	N-CA-C	-5.29	105.63	111.71
1	B	81	PRO	N-CA-C	5.28	123.36	112.47
1	B	699	LYS	N-CA-C	-5.27	105.53	111.28
3	D	29	ALA	N-CA-C	-5.26	105.66	111.71
4	E	30	GLY	N-CA-C	-5.26	106.32	113.37
1	A	121	GLY	N-CA-C	-5.26	107.86	115.27
4	F	30	GLY	N-CA-C	-5.26	106.33	113.37
2	G	328	ALA	N-CA-C	-5.24	106.59	112.87
2	H	328	ALA	N-CA-C	-5.22	106.60	112.87
2	H	289	LEU	CA-C-N	-5.21	111.82	120.68
2	H	289	LEU	C-N-CA	-5.21	111.82	120.68
1	A	640	ALA	N-CA-C	5.21	118.79	112.23
1	A	623	LEU	N-CA-C	-5.19	106.90	113.18
1	B	749	LEU	N-CA-C	-5.19	106.25	112.58
1	A	134	ALA	N-CA-C	-5.18	105.63	111.28
1	A	266	MET	N-CA-C	-5.18	105.63	111.28
2	G	289	LEU	CA-C-N	-5.18	111.88	120.68
2	G	289	LEU	C-N-CA	-5.18	111.88	120.68
2	H	234	TYR	N-CA-C	-5.17	99.78	110.80
1	A	749	LEU	N-CA-C	-5.17	106.28	112.58
1	B	266	MET	N-CA-C	-5.16	105.66	111.28
2	G	234	TYR	N-CA-C	-5.15	99.82	110.80
1	B	640	ALA	N-CA-C	5.15	118.72	112.23
1	B	86	LEU	N-CA-C	-5.15	105.56	111.07
1	B	134	ALA	N-CA-C	-5.15	105.67	111.28
2	G	157	ILE	CA-C-N	-5.14	112.49	120.31
2	G	157	ILE	C-N-CA	-5.14	112.49	120.31
1	A	86	LEU	N-CA-C	-5.10	105.61	111.07
2	H	157	ILE	CA-C-N	-5.10	112.55	120.31
2	H	157	ILE	C-N-CA	-5.10	112.55	120.31
1	A	93	HIS	N-CA-C	-5.07	105.88	111.71
2	H	199	ASN	N-CA-C	-5.07	106.93	113.01
1	B	660	LEU	CA-C-N	-5.04	114.21	120.56
1	B	660	LEU	C-N-CA	-5.04	114.21	120.56
2	H	99	ARG	CA-C-N	-5.04	114.11	122.92
2	H	99	ARG	C-N-CA	-5.04	114.11	122.92
1	A	765	GLU	N-CA-C	-5.03	105.25	111.33
2	G	99	ARG	CA-C-N	-5.02	114.13	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	99	ARG	C-N-CA	-5.02	114.13	122.92
1	B	739	HIS	N-CA-C	-5.02	105.94	111.71

There are no chirality outliers.

There are no planarity outliers.

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	3092	0	856	24	0
1	B	3092	0	856	17	0
2	G	1624	0	446	22	0
2	H	1624	0	446	16	0
3	C	140	0	36	0	0
3	D	140	0	36	0	0
4	E	260	0	86	1	0
4	F	260	0	86	1	0
All	All	10232	0	2848	71	0

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 5.

All (71) 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:A:776:MET:O	1:B:778:ALA:O	1.54	1.25
1:A:776:MET:O	1:B:778:ALA:C	1.98	1.06
1:A:778:ALA:C	1:B:776:MET:O	1.99	1.04
1:A:778:ALA:O	1:B:776:MET:O	1.83	0.95
2:H:103:GLU:H	2:H:108:GLY:HA3	1.39	0.86
2:G:103:GLU:H	2:G:108:GLY:HA3	1.39	0.85
1:A:726:ASP:O	2:G:258:GLY:CA	2.29	0.80
1:A:726:ASP:O	2:G:258:GLY:HA2	1.84	0.77
2:H:103:GLU:H	2:H:108:GLY:CA	2.03	0.72
2:G:103:GLU:H	2:G:108:GLY:CA	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ASP:C	2:G:258:GLY:HA2	2.16	0.70
2:G:56:PHE:O	2:G:63:SER:C	2.42	0.63
2:H:56:PHE:O	2:H:63:SER:C	2.42	0.62
1:A:726:ASP:O	2:G:258:GLY:HA3	2.00	0.62
2:H:57:ALA:O	2:H:59:TYR:N	2.33	0.62
2:G:57:ALA:O	2:G:59:TYR:N	2.33	0.61
1:B:103:GLY:H	1:B:529:GLN:H	1.47	0.61
2:H:56:PHE:O	2:H:63:SER:CA	2.48	0.61
2:G:56:PHE:O	2:G:63:SER:CA	2.48	0.60
1:A:103:GLY:H	1:A:529:GLN:H	1.47	0.59
2:G:343:ALA:O	2:G:349:GLY:HA3	2.03	0.58
2:H:57:ALA:O	2:H:58:LEU:C	2.46	0.58
2:H:343:ALA:O	2:H:349:GLY:HA3	2.03	0.58
1:A:500:LYS:CA	1:A:504:GLY:HA2	2.35	0.57
2:G:57:ALA:O	2:G:58:LEU:C	2.46	0.56
1:B:500:LYS:CA	1:B:504:GLY:HA2	2.35	0.56
1:B:103:GLY:N	1:B:529:GLN:H	2.09	0.51
1:A:778:ALA:CA	1:B:776:MET:O	2.59	0.50
1:A:103:GLY:N	1:A:529:GLN:H	2.09	0.50
4:E:44:VAL:C	4:E:46:GLY:H	2.20	0.50
1:A:331:GLU:N	2:G:253:ARG:O	2.35	0.49
1:A:411:MET:C	1:A:413:GLY:H	2.21	0.49
4:F:44:VAL:C	4:F:46:GLY:H	2.20	0.49
1:B:411:MET:C	1:B:413:GLY:H	2.21	0.48
1:B:123:GLY:HA2	1:B:171:ASP:O	2.14	0.47
2:H:103:GLU:N	2:H:108:GLY:HA3	2.20	0.47
1:A:123:GLY:HA2	1:A:171:ASP:O	2.14	0.47
2:G:103:GLU:N	2:G:108:GLY:HA3	2.20	0.47
2:G:234:TYR:C	2:G:236:GLN:H	2.23	0.47
1:A:528:ARG:C	1:A:530:GLY:H	2.24	0.45
2:H:234:TYR:C	2:H:236:GLN:H	2.23	0.45
1:B:85:GLN:C	1:B:88:GLY:H	2.25	0.45
2:G:234:TYR:C	2:G:236:GLN:N	2.74	0.45
2:H:232:ILE:C	2:H:234:TYR:N	2.74	0.45
2:H:234:TYR:C	2:H:236:GLN:N	2.74	0.45
1:B:528:ARG:C	1:B:530:GLY:H	2.24	0.44
1:A:85:GLN:C	1:A:88:GLY:H	2.25	0.44
2:G:232:ILE:C	2:G:234:TYR:N	2.74	0.44
2:G:153:SER:C	2:G:155:ILE:N	2.73	0.44
2:H:62:PHE:O	2:H:63:SER:O	2.35	0.44
2:G:62:PHE:O	2:G:63:SER:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:C	1:A:256:THR:H	2.26	0.44
1:B:254:ILE:C	1:B:256:THR:H	2.26	0.44
2:H:214:GLY:C	2:H:216:LEU:H	2.26	0.44
1:B:497:GLU:C	1:B:499:VAL:H	2.25	0.43
2:H:161:THR:O	2:H:165:GLY:HA3	2.19	0.43
2:G:161:THR:O	2:G:165:GLY:HA3	2.19	0.43
1:A:497:GLU:C	1:A:499:VAL:H	2.26	0.42
1:A:499:VAL:C	1:A:501:GLU:H	2.28	0.42
2:G:214:GLY:C	2:G:216:LEU:H	2.26	0.42
2:G:215:PRO:C	2:G:217:THR:N	2.75	0.42
1:A:105:GLY:O	1:A:107:THR:N	2.50	0.42
1:A:524:GLY:C	1:A:526:SER:H	2.28	0.42
2:G:385:ILE:C	2:G:387:VAL:H	2.28	0.41
2:H:385:ILE:C	2:H:387:VAL:H	2.28	0.41
1:B:105:GLY:O	1:B:107:THR:N	2.50	0.41
1:B:524:GLY:C	1:B:526:SER:H	2.28	0.41
2:H:215:PRO:C	2:H:217:THR:N	2.75	0.41
1:B:499:VAL:C	1:B:501:GLU:H	2.28	0.41
1:A:357:PHE:O	1:A:361:PHE:N	2.54	0.40
1:A:209:VAL:C	1:A:211:SER:N	2.78	0.40

There are no symmetry-related clashes.

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	771/779 (99%)	638 (83%)	86 (11%)	47 (6%)	1	13
1	B	771/779 (99%)	638 (83%)	85 (11%)	48 (6%)	1	13
2	G	402/429 (94%)	321 (80%)	52 (13%)	29 (7%)	1	11
2	H	402/429 (94%)	319 (79%)	54 (13%)	29 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	33/65 (51%)	33 (100%)	0	0	100	100
3	D	33/65 (51%)	33 (100%)	0	0	100	100
4	E	63/107 (59%)	57 (90%)	5 (8%)	1 (2%)	7	38
4	F	63/107 (59%)	57 (90%)	5 (8%)	1 (2%)	7	38
All	All	2538/2760 (92%)	2096 (83%)	287 (11%)	155 (6%)	1	13

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	80	PHE
1	A	99	GLU
1	A	100	MET
1	A	101	LYS
1	A	197	VAL
1	A	306	TYR
1	A	326	GLY
1	A	371	THR
1	A	543	ASP
1	A	570	GLN
1	A	645	ARG
1	A	649	PRO
1	A	650	GLU
1	A	744	ALA
1	B	36	LEU
1	B	80	PHE
1	B	99	GLU
1	B	100	MET
1	B	101	LYS
1	B	197	VAL
1	B	306	TYR
1	B	326	GLY
1	B	371	THR
1	B	543	ASP
1	B	570	GLN
1	B	645	ARG
1	B	649	PRO
1	B	650	GLU
1	B	744	ALA
2	G	36	ILE
2	G	37	PRO

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Mol	Chain	Res	Type
2	G	58	LEU
2	G	63	SER
2	G	236	GLN
2	G	347	ILE
2	G	350	VAL
2	H	36	ILE
2	H	37	PRO
2	H	58	LEU
2	H	63	SER
2	H	236	GLN
2	H	347	ILE
2	H	350	VAL
1	A	8	MET
1	A	102	THR
1	A	104	GLU
1	A	198	GLN
1	A	252	TYR
1	A	351	THR
1	A	410	THR
1	A	477	LYS
1	A	490	GLY
1	A	676	ILE
1	B	8	MET
1	B	102	THR
1	B	104	GLU
1	B	198	GLN
1	B	252	TYR
1	B	351	THR
1	B	410	THR
1	B	477	LYS
1	B	490	GLY
1	B	676	ILE
2	G	181	ILE
2	G	237	GLU
2	G	257	ALA
2	G	340	LEU
2	G	419	ILE
2	H	181	ILE
2	H	237	GLU
2	H	257	ALA
2	H	340	LEU
2	H	419	ILE

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Mol	Chain	Res	Type
4	E	40	SER
4	F	40	SER
1	A	187	ASP
1	A	262	THR
1	A	323	LEU
1	A	493	ILE
1	A	511	GLU
1	A	565	ASP
1	A	678	GLY
1	B	187	ASP
1	B	262	THR
1	B	323	LEU
1	B	493	ILE
1	B	511	GLU
1	B	565	ASP
1	B	678	GLY
2	G	13	GLU
2	G	207	LYS
2	G	234	TYR
2	G	329	VAL
2	G	345	ALA
2	H	13	GLU
2	H	207	LYS
2	H	234	TYR
2	H	329	VAL
2	H	345	ALA
1	A	77	THR
1	A	96	ASN
1	A	162	ASP
1	A	273	PHE
1	A	365	GLU
1	A	386	ASN
1	A	745	GLN
1	B	77	THR
1	B	96	ASN
1	B	162	ASP
1	B	200	PRO
1	B	273	PHE
1	B	365	GLU
1	B	386	ASN
1	B	745	GLN
2	G	150	PRO

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Mol	Chain	Res	Type
2	G	153	SER
2	G	205	TYR
2	G	269	PRO
2	G	272	VAL
2	H	150	PRO
2	H	153	SER
2	H	205	TYR
2	H	269	PRO
2	H	272	VAL
1	A	200	PRO
1	A	318	SER
1	A	411	MET
1	B	318	SER
1	B	411	MET
2	G	76	GLY
2	G	141	PRO
2	G	243	PRO
2	G	386	SER
2	G	397	GLY
2	H	76	GLY
2	H	141	PRO
2	H	243	PRO
2	H	386	SER
2	H	397	GLY
1	A	105	GLY
1	A	215	ASP
1	B	105	GLY
1	B	171	ASP
1	B	215	ASP
2	G	68	GLY
2	H	68	GLY
1	A	97	ILE
1	A	396	ARG
1	B	97	ILE
1	B	396	ARG
1	A	190	VAL
1	B	190	VAL
2	G	34	ILE
2	H	34	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	773/779 (99%)	5.91	715 (92%) 0 1	321, 444, 550, 648	0
1	B	773/779 (99%)	6.63	722 (93%) 0 1	340, 470, 540, 612	0
2	G	406/429 (94%)	5.65	362 (89%) 0 1	321, 409, 488, 512	0
2	H	406/429 (94%)	5.73	366 (90%) 0 1	372, 466, 536, 558	0
3	C	35/65 (53%)	4.68	33 (94%) 0 1	328, 363, 402, 405	0
3	D	35/65 (53%)	5.17	31 (88%) 0 1	383, 396, 463, 466	0
4	E	65/107 (60%)	4.61	52 (80%) 0 1	386, 446, 468, 473	0
4	F	65/107 (60%)	4.67	51 (78%) 0 1	477, 523, 550, 551	0
All	All	2558/2760 (92%)	5.97	2332 (91%) 0 1	321, 450, 541, 648	0

All (2332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	642	TYR	48.7
1	B	81	PRO	31.9
1	B	394	THR	30.6
1	B	231	THR	28.2
2	G	140	SER	27.1
2	H	212	ASP	26.5
1	B	479	ALA	26.2
1	B	561	PHE	26.1
2	H	255	LEU	25.9
2	G	426	TYR	25.3
1	B	533	GLY	25.2
1	A	658	VAL	25.0
1	B	529	GLN	25.0
1	A	647	GLU	24.5
1	B	644	PRO	24.4
1	A	276	ASP	24.2

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Mol	Chain	Res	Type	RSRZ
2	H	122	PHE	23.8
1	B	395	ASN	23.7
1	B	667	ASP	23.7
1	B	483	ALA	22.4
1	B	373	THR	22.4
1	B	234	TYR	22.3
1	B	478	GLY	21.8
1	B	57	THR	21.7
1	A	646	GLU	21.5
2	G	258	GLY	21.4
2	G	338	GLU	21.1
1	B	56	ALA	21.1
1	B	54	LYS	21.1
2	H	160	LEU	21.1
1	B	493	ILE	21.1
1	B	235	VAL	21.0
1	A	536	GLN	21.0
1	A	363	MET	21.0
1	B	103	GLY	20.3
1	A	656	GLY	19.9
1	B	216	GLU	19.7
2	G	105	GLY	19.6
1	A	665	TYR	19.6
1	B	258	ALA	19.6
2	H	299	VAL	19.6
1	B	534	ILE	19.4
1	A	501	GLU	19.1
1	A	277	ASN	19.1
1	B	492	ASP	18.9
1	A	679	LYS	18.9
1	B	560	ARG	18.8
4	E	38	GLY	18.7
2	H	106	ASP	18.6
1	B	497	GLU	18.5
2	G	264	PRO	18.2
2	G	301	ALA	18.2
2	G	351	ARG	18.0
1	A	32	ASP	17.9
1	B	673	LYS	17.8
2	H	214	GLY	17.8
2	H	210	THR	17.7
1	B	650	GLU	17.4

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Mol	Chain	Res	Type	RSRZ
2	H	300	ILE	17.3
1	A	76	VAL	17.1
1	B	476	GLN	17.1
1	A	427	MET	17.1
1	B	564	ASP	16.9
1	B	309	GLU	16.9
2	G	368	ILE	16.8
2	H	274	PRO	16.8
1	B	477	LYS	16.7
1	A	362	ARG	16.7
1	A	678	GLY	16.5
1	B	278	LEU	16.5
2	H	67	LEU	16.5
2	G	427	VAL	16.4
1	B	551	ALA	16.2
2	G	67	LEU	16.2
1	B	510	THR	16.2
2	H	71	THR	16.2
1	B	643	THR	16.1
2	H	213	ILE	16.1
2	H	161	THR	16.0
2	H	388	TRP	16.0
1	B	156	LEU	15.8
1	B	105	GLY	15.7
1	A	663	THR	15.7
1	A	664	THR	15.7
1	A	701	GLU	15.6
1	B	107	THR	15.5
1	B	540	SER	15.5
1	B	451	ASN	15.5
1	B	346	GLN	15.4
1	B	739	HIS	15.3
1	A	247	GLU	15.2
1	A	659	ASP	15.2
1	B	328	ARG	15.1
3	D	53	LYS	15.0
1	B	53	GLU	15.0
3	D	54	ILE	14.9
1	B	217	ALA	14.8
2	H	420	GLN	14.6
2	H	107	TYR	14.6
1	B	259	VAL	14.5

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Mol	Chain	Res	Type	RSRZ
1	B	581	SER	14.5
2	G	292	VAL	14.4
1	B	196	MET	14.4
1	B	347	ASN	14.3
2	H	190	PHE	14.3
1	A	697	ASN	14.3
1	B	503	GLY	14.2
1	A	496	GLY	14.2
1	B	674	SER	14.1
1	B	535	THR	14.1
2	G	288	LEU	14.0
1	A	250	TYR	13.9
1	A	642	TYR	13.9
1	B	197	VAL	13.9
4	F	25	GLY	13.8
1	A	704	GLY	13.8
1	B	336	ALA	13.8
1	B	678	GLY	13.8
1	B	157	ASN	13.7
1	A	354	THR	13.7
2	G	428	ARG	13.7
1	A	249	ASP	13.7
1	B	428	THR	13.6
1	B	132	TYR	13.6
2	H	254	GLN	13.5
2	H	389	PHE	13.4
2	G	201	VAL	13.4
2	H	260	LYS	13.4
2	G	102	LYS	13.4
1	A	315	ILE	13.3
1	B	427	MET	13.3
1	B	528	ARG	13.3
1	B	562	GLY	13.2
1	B	589	ASN	13.2
1	A	476	GLN	13.2
1	A	674	SER	13.1
1	A	712	GLU	13.0
2	H	292	VAL	12.9
1	B	253	ASP	12.9
1	A	535	THR	12.8
3	D	52	THR	12.7
1	A	696	TYR	12.7

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Mol	Chain	Res	Type	RSRZ
1	B	482	ILE	12.7
4	F	27	GLY	12.6
1	A	346	GLN	12.6
2	G	261	THR	12.5
1	B	430	GLN	12.5
1	B	31	GLY	12.5
1	B	102	THR	12.5
1	B	131	GLU	12.5
2	H	203	GLN	12.5
1	B	549	PHE	12.4
2	G	139	VAL	12.4
1	B	181	GLY	12.3
1	B	130	ASN	12.3
1	A	591	ASP	12.3
1	A	620	SER	12.3
1	A	259	VAL	12.2
1	B	714	VAL	12.2
2	H	301	ALA	12.1
2	H	422	LYS	12.1
4	F	29	VAL	12.1
1	B	688	ILE	12.1
1	B	121	GLY	12.0
2	G	183	ASN	12.0
1	A	278	LEU	12.0
1	B	550	GLY	12.0
1	B	457	GLN	12.0
1	B	563	MET	12.0
1	A	666	LEU	12.0
2	H	317	THR	12.0
1	A	468	ALA	12.0
1	B	104	GLU	12.0
1	A	275	ILE	12.0
2	H	147	VAL	11.9
1	A	75	ARG	11.9
2	H	128	SER	11.9
2	G	257	ALA	11.9
1	A	171	ASP	11.8
1	A	295	LYS	11.8
1	B	397	PRO	11.8
1	B	32	ASP	11.8
1	A	161	LYS	11.8
1	B	359	ASN	11.7

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Mol	Chain	Res	Type	RSRZ
1	B	547	ARG	11.7
2	H	288	LEU	11.7
2	H	150	PRO	11.7
2	H	395	PHE	11.7
1	A	744	ALA	11.7
4	E	39	GLN	11.6
1	A	694	THR	11.6
1	B	271	LYS	11.5
2	G	350	VAL	11.5
1	B	539	LEU	11.5
2	G	202	ILE	11.4
2	G	259	ARG	11.4
1	A	430	GLN	11.4
2	G	243	PRO	11.4
1	A	643	THR	11.4
2	G	101	ALA	11.4
1	A	455	PRO	11.4
1	B	161	LYS	11.3
2	G	125	THR	11.3
2	G	106	ASP	11.3
2	H	202	ILE	11.3
2	H	211	GLY	11.3
1	A	66	PHE	11.3
1	A	714	VAL	11.3
2	G	98	GLN	11.2
2	H	90	LEU	11.2
1	B	675	ASP	11.2
2	G	107	TYR	11.2
2	G	104	GLU	11.1
4	E	45	GLY	11.1
2	H	387	VAL	11.1
2	H	293	GLN	11.1
2	G	260	LYS	11.1
1	B	355	ILE	11.1
2	H	259	ARG	11.1
1	A	410	THR	11.1
2	G	337	ALA	11.1
1	A	153	GLY	11.1
1	B	690	ASP	11.0
2	H	115	TYR	11.0
3	C	29	ALA	11.0
1	B	33	TYR	11.0

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Mol	Chain	Res	Type	RSRZ
1	A	653	LYS	11.0
2	G	423	TYR	11.0
4	E	46	GLY	11.0
1	A	529	GLN	11.0
1	A	662	ASN	10.9
2	H	276	ILE	10.9
1	A	668	GLU	10.9
1	A	355	ILE	10.9
2	G	66	ASN	10.9
2	H	419	ILE	10.9
1	B	408	TYR	10.9
2	G	374	PHE	10.8
1	B	740	LEU	10.8
1	A	673	LYS	10.8
1	A	700	GLU	10.8
1	B	484	THR	10.8
1	A	20	GLU	10.8
1	A	104	GLU	10.8
1	B	679	LYS	10.8
1	A	654	LEU	10.8
1	B	71	GLU	10.7
1	B	704	GLY	10.7
1	B	435	GLY	10.7
1	B	64	GLU	10.7
2	H	355	ASP	10.7
1	B	652	TRP	10.7
1	A	279	PHE	10.7
1	A	571	SER	10.7
4	F	31	ALA	10.7
2	H	66	ASN	10.6
1	A	85	GLN	10.6
1	B	605	GLN	10.6
1	B	456	HIS	10.6
2	H	318	PHE	10.6
2	H	68	GLY	10.6
1	A	409	ARG	10.6
1	B	556	ALA	10.5
1	B	649	PRO	10.5
1	B	401	ASP	10.5
1	B	155	ASN	10.5
4	E	33	PHE	10.5
1	A	502	LEU	10.5

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLY	10.5
2	H	146	VAL	10.5
1	B	118	ALA	10.4
1	A	530	GLY	10.4
2	G	252	GLY	10.4
1	A	313	VAL	10.4
1	B	565	ASP	10.4
1	A	197	VAL	10.4
1	B	205	VAL	10.4
1	A	244	LEU	10.4
1	A	661	ILE	10.3
1	A	472	GLU	10.3
1	B	256	THR	10.3
1	B	684	MET	10.3
1	B	668	GLU	10.3
2	G	341	HIS	10.3
1	B	171	ASP	10.3
2	H	386	SER	10.3
4	E	32	ALA	10.3
1	A	373	THR	10.2
2	H	98	GLN	10.2
2	H	315	TYR	10.2
2	H	141	PRO	10.2
1	A	196	MET	10.2
1	A	652	TRP	10.2
1	B	490	GLY	10.2
1	B	426	TYR	10.2
1	A	655	ASP	10.2
1	B	277	ASN	10.1
2	H	286	SER	10.1
4	F	35	GLY	10.1
1	A	657	LEU	10.1
2	G	27	ILE	10.1
1	A	575	SER	10.1
2	H	118	TYR	10.1
2	G	409	ASP	10.1
2	H	365	ASN	10.1
1	A	124	VAL	10.1
1	A	752	TYR	10.0
1	B	124	VAL	10.0
2	H	297	ILE	10.0
1	A	693	ILE	10.0

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Mol	Chain	Res	Type	RSRZ
2	G	141	PRO	10.0
3	D	55	ILE	10.0
1	A	130	ASN	10.0
1	A	347	ASN	10.0
2	H	125	THR	10.0
1	B	455	PRO	10.0
2	G	8	LEU	9.9
2	H	302	ASP	9.9
1	B	122	LYS	9.9
2	G	352	PRO	9.9
1	B	713	LYS	9.9
1	A	31	GLY	9.9
4	F	28	ASP	9.9
1	B	179	GLU	9.9
1	B	715	ILE	9.9
1	A	531	ASP	9.9
1	B	501	GLU	9.9
1	B	597	LEU	9.9
1	B	337	ILE	9.9
2	H	174	ASP	9.8
2	H	346	PHE	9.8
2	G	172	ILE	9.8
2	H	126	VAL	9.8
4	E	10	VAL	9.8
1	A	252	TYR	9.8
2	H	350	VAL	9.8
1	A	35	ASN	9.7
1	B	232	LYS	9.7
1	B	653	LYS	9.7
1	B	371	THR	9.7
2	G	124	ALA	9.7
2	G	321	PHE	9.7
1	A	395	ASN	9.7
1	A	67	ALA	9.7
1	A	169	ALA	9.7
1	B	52	LEU	9.7
1	A	428	THR	9.7
1	B	664	THR	9.7
1	A	605	GLN	9.6
1	A	667	ASP	9.6
2	G	291	PHE	9.6
2	G	298	LYS	9.6

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Mol	Chain	Res	Type	RSRZ
2	H	298	LYS	9.6
1	B	546	MET	9.6
1	A	33	TYR	9.6
2	G	395	PHE	9.6
1	B	438	ALA	9.6
1	A	454	ILE	9.6
1	B	160	SER	9.6
1	B	651	GLU	9.6
2	G	270	ALA	9.6
1	B	569	ILE	9.6
2	G	240	ARG	9.6
2	G	212	ASP	9.6
3	D	46	ILE	9.6
1	B	718	ARG	9.6
2	G	128	SER	9.6
2	G	241	ARG	9.5
1	B	388	GLN	9.5
2	G	161	THR	9.5
2	G	339	ASN	9.5
2	G	31	GLY	9.5
1	A	264	GLU	9.5
1	B	548	ARG	9.5
1	B	585	VAL	9.5
2	G	126	VAL	9.5
1	A	170	ALA	9.5
1	B	621	GLU	9.5
1	B	622	ASN	9.5
1	B	412	GLU	9.5
1	B	198	GLN	9.4
2	H	425	SER	9.4
2	G	100	LEU	9.4
4	F	36	GLY	9.3
1	B	726	ASP	9.3
2	G	376	SER	9.3
2	G	195	ALA	9.3
2	H	8	LEU	9.3
1	A	368	ALA	9.3
2	H	282	LEU	9.3
1	B	423	ALA	9.3
2	H	204	PHE	9.3
1	A	84	VAL	9.3
1	B	586	GLU	9.3

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Mol	Chain	Res	Type	RSRZ
2	H	296	PHE	9.3
1	A	102	THR	9.2
1	B	472	GLU	9.2
1	B	393	PRO	9.2
2	G	147	VAL	9.2
1	A	453	GLY	9.2
2	G	148	GLU	9.2
1	B	303	ASP	9.2
2	H	154	PHE	9.1
1	A	533	GLY	9.1
1	A	534	ILE	9.1
1	B	749	LEU	9.1
1	A	132	TYR	9.1
2	G	315	TYR	9.1
4	F	40	SER	9.1
1	A	173	THR	9.0
1	B	252	TYR	9.0
2	G	349	GLY	9.0
1	A	280	ASP	9.0
1	A	299	ALA	9.0
1	A	438	ALA	9.0
1	B	343	LEU	9.0
2	H	421	LYS	9.0
2	G	206	GLU	9.0
1	B	424	GLN	9.0
1	B	76	VAL	9.0
1	B	458	VAL	9.0
1	B	310	ASP	9.0
2	G	59	TYR	9.0
1	A	292	GLN	9.0
1	A	385	TYR	9.0
1	A	176	THR	8.9
1	B	770	GLU	8.9
2	G	114	GLU	8.9
4	F	20	THR	8.9
1	A	69	VAL	8.9
1	A	156	LEU	8.9
1	B	639	ILE	8.9
2	G	167	MET	8.9
2	H	273	ILE	8.9
1	A	386	ASN	8.9
1	B	498	GLY	8.9

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Mol	Chain	Res	Type	RSRZ
4	F	32	ALA	8.9
2	G	99	ARG	8.9
1	A	540	SER	8.8
1	A	174	TYR	8.8
1	A	129	VAL	8.8
1	A	359	ASN	8.8
1	A	625	GLU	8.8
1	B	628	GLU	8.8
2	H	316	VAL	8.8
1	B	491	THR	8.8
1	A	490	GLY	8.8
1	A	291	ASN	8.8
1	B	641	ALA	8.7
1	B	162	ASP	8.7
1	B	721	ASP	8.7
1	A	40	ALA	8.7
1	A	506	ALA	8.7
2	G	173	ALA	8.7
2	G	383	ILE	8.7
3	C	54	ILE	8.7
1	B	431	PRO	8.7
1	A	353	ALA	8.7
2	H	193	ILE	8.6
1	A	157	ASN	8.6
1	B	669	GLY	8.6
2	G	293	GLN	8.6
1	B	175	SER	8.6
1	B	100	MET	8.6
1	A	118	ALA	8.6
2	G	115	TYR	8.6
1	B	707	GLN	8.6
1	B	218	ARG	8.6
1	B	454	ILE	8.6
1	A	162	ASP	8.6
2	G	290	ASN	8.5
2	H	290	ASN	8.5
1	A	702	GLN	8.5
2	H	374	PHE	8.5
1	A	484	THR	8.5
1	B	629	ASN	8.4
1	B	405	ASP	8.4
1	A	258	ALA	8.4

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Mol	Chain	Res	Type	RSRZ
2	H	148	GLU	8.4
2	G	58	LEU	8.4
1	B	106	LYS	8.4
1	B	453	GLY	8.4
1	A	175	SER	8.4
1	A	680	GLU	8.4
1	B	738	ILE	8.4
2	G	387	VAL	8.4
2	G	127	GLN	8.4
2	G	25	PHE	8.4
1	B	399	VAL	8.3
1	A	65	ALA	8.3
1	B	415	PHE	8.3
1	A	305	ASP	8.3
1	A	651	GLU	8.3
1	B	429	GLY	8.3
2	G	150	PRO	8.3
2	G	205	TYR	8.3
1	A	38	ASP	8.3
2	G	223	ALA	8.3
1	B	219	THR	8.3
1	A	253	ASP	8.3
1	B	434	VAL	8.3
1	A	705	LYS	8.3
1	B	305	ASP	8.2
1	B	176	THR	8.2
1	B	314	VAL	8.2
1	B	55	GLY	8.2
3	C	60	SER	8.2
2	G	299	VAL	8.2
2	H	89	LEU	8.2
1	A	234	TYR	8.2
1	B	236	GLN	8.2
1	B	142	GLY	8.2
2	H	351	ARG	8.2
3	D	35	ILE	8.2
1	B	220	PRO	8.2
1	B	247	GLU	8.2
1	A	733	GLN	8.2
1	A	497	GLU	8.1
1	B	753	GLN	8.1
1	A	460	ASN	8.1

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Mol	Chain	Res	Type	RSRZ
2	G	118	TYR	8.1
1	B	658	VAL	8.1
1	A	442	SER	8.1
1	A	639	ILE	8.1
2	H	401	LEU	8.1
1	A	246	ALA	8.1
1	B	165	ARG	8.1
2	H	142	LYS	8.1
1	A	491	THR	8.1
1	A	142	GLY	8.1
1	A	592	SER	8.1
1	B	746	THR	8.1
1	B	689	MET	8.1
1	A	616	GLU	8.1
1	B	646	GLU	8.1
1	A	372	GLY	8.1
1	A	248	LYS	8.1
1	B	200	PRO	8.0
1	B	353	ALA	8.0
4	E	37	MET	8.0
3	D	49	LEU	8.0
1	A	82	PHE	8.0
1	A	528	ARG	8.0
1	A	223	ILE	8.0
4	F	37	MET	8.0
1	B	432	VAL	8.0
1	B	672	GLU	8.0
2	G	340	LEU	8.0
2	H	256	TYR	8.0
2	H	109	ARG	8.0
1	B	752	TYR	7.9
2	H	289	LEU	7.9
1	A	329	TYR	7.9
1	A	100	MET	7.9
2	G	111	LYS	7.9
1	A	580	SER	7.9
1	A	345	ILE	7.9
1	A	238	ASN	7.9
1	A	351	THR	7.9
2	G	162	LEU	7.9
1	A	336	ALA	7.9
4	E	31	ALA	7.9

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Mol	Chain	Res	Type	RSRZ
1	B	591	ASP	7.9
2	G	322	PHE	7.9
1	A	294	LEU	7.9
1	A	178	ASN	7.9
1	B	129	VAL	7.9
2	G	263	LEU	7.9
2	H	180	GLY	7.9
2	G	416	THR	7.9
1	B	572	LYS	7.9
2	H	168	PHE	7.9
1	B	588	ASN	7.8
4	E	29	VAL	7.8
1	A	6	ASN	7.8
2	H	428	ARG	7.8
1	B	374	ALA	7.8
2	G	323	THR	7.8
1	A	707	GLN	7.8
2	G	244	ILE	7.8
1	A	660	LEU	7.7
1	B	573	MET	7.7
2	H	30	LEU	7.7
2	H	226	ILE	7.7
2	G	425	SER	7.7
1	A	72	ALA	7.7
1	A	103	GLY	7.7
1	B	407	ILE	7.7
1	B	159	MET	7.7
1	B	530	GLY	7.7
2	H	137	GLY	7.7
1	A	514	GLU	7.7
1	B	600	ASP	7.7
2	H	155	ILE	7.7
2	H	183	ASN	7.7
4	F	19	SER	7.7
1	B	583	LYS	7.6
1	A	296	ALA	7.6
1	B	169	ALA	7.6
1	B	296	ALA	7.6
1	A	123	GLY	7.6
2	G	182	GLY	7.6
2	H	99	ARG	7.6
2	H	96	SER	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	270	GLU	7.6
1	B	195	GLN	7.6
2	G	316	VAL	7.6
1	B	708	MET	7.6
1	A	320	THR	7.6
2	G	365	ASN	7.6
2	H	72	VAL	7.6
1	A	19	TYR	7.6
1	A	757	PHE	7.6
1	A	500	LYS	7.6
1	B	215	ASP	7.6
1	A	349	SER	7.6
1	A	617	VAL	7.6
2	H	105	GLY	7.6
1	A	154	LEU	7.6
1	A	168	TYR	7.6
2	H	426	TYR	7.6
1	B	281	VAL	7.6
1	A	30	ARG	7.5
2	G	95	PRO	7.5
2	H	390	ASN	7.5
1	A	464	HIS	7.5
3	D	36	PHE	7.5
1	A	589	ASN	7.5
1	A	473	GLU	7.5
1	B	335	GLN	7.5
1	A	107	THR	7.5
1	A	633	SER	7.5
1	B	238	ASN	7.5
1	B	697	ASN	7.5
1	A	152	VAL	7.5
1	B	686	GLU	7.5
1	A	495	LEU	7.5
1	A	328	ARG	7.5
1	B	120	THR	7.4
1	B	244	LEU	7.4
1	A	71	GLU	7.4
2	G	96	SER	7.4
2	G	74	ALA	7.4
1	A	632	LYS	7.4
1	B	571	SER	7.4
1	A	155	ASN	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	125	HIS	7.4
4	E	34	GLY	7.4
1	B	239	ALA	7.4
1	B	75	ARG	7.4
1	B	65	ALA	7.4
1	A	586	GLU	7.4
1	A	672	GLU	7.4
2	G	420	GLN	7.4
1	B	135	SER	7.4
2	H	294	ASN	7.4
1	A	260	GLN	7.4
2	H	172	ILE	7.4
1	A	251	THR	7.4
1	B	509	GLY	7.4
2	G	151	GLY	7.4
1	B	199	ARG	7.4
1	A	753	GLN	7.3
2	G	163	VAL	7.3
2	H	372	ALA	7.3
4	F	30	GLY	7.3
1	B	243	THR	7.3
1	B	93	HIS	7.3
2	G	198	PRO	7.3
2	G	348	PRO	7.3
1	B	386	ASN	7.3
1	A	737	GLY	7.3
1	B	709	ARG	7.3
1	B	45	THR	7.3
1	A	507	VAL	7.3
1	B	80	PHE	7.3
1	A	268	LYS	7.3
1	A	539	LEU	7.3
2	H	295	PRO	7.3
1	A	172	ILE	7.3
1	B	532	PRO	7.2
1	B	249	ASP	7.2
4	E	24	LYS	7.2
1	A	179	GLU	7.2
1	B	260	GLN	7.2
1	A	467	GLU	7.2
1	B	719	ALA	7.2
1	A	527	GLY	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	70	ARG	7.2
2	H	206	GLU	7.2
1	A	257	LYS	7.2
1	A	144	ILE	7.2
1	B	691	ARG	7.2
1	A	300	MET	7.2
1	B	368	ALA	7.2
1	A	671	LEU	7.2
1	B	136	ARG	7.2
1	B	48	PHE	7.2
1	A	624	ARG	7.2
1	B	511	GLU	7.2
2	G	196	ASN	7.2
1	B	716	VAL	7.1
2	H	399	THR	7.1
1	A	236	GLN	7.1
1	B	524	GLY	7.1
2	G	371	GLY	7.1
1	B	545	LEU	7.1
2	H	375	LEU	7.1
2	H	240	ARG	7.1
1	B	166	GLU	7.1
1	A	357	PHE	7.1
1	B	775	VAL	7.1
2	H	209	LYS	7.1
2	H	173	ALA	7.1
1	A	151	THR	7.1
2	G	239	GLU	7.1
3	D	45	TRP	7.1
1	B	350	MET	7.1
2	G	180	GLY	7.1
1	A	408	TYR	7.1
2	G	164	ALA	7.1
1	B	302	LYS	7.1
1	B	741	ARG	7.1
1	A	77	THR	7.1
1	A	166	GLU	7.1
2	H	246	TYR	7.1
1	B	297	HIS	7.1
2	H	331	ILE	7.1
1	B	469	GLN	7.0
2	H	379	ALA	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	233	LEU	7.0
2	G	204	PHE	7.0
2	H	322	PHE	7.0
2	H	291	PHE	7.0
1	B	598	GLN	7.0
2	H	287	THR	7.0
1	A	543	ASP	7.0
2	H	268	ASN	7.0
2	G	382	PRO	7.0
1	B	372	GLY	7.0
2	G	213	ILE	7.0
1	A	218	ARG	7.0
1	A	548	ARG	7.0
2	G	373	LEU	7.0
1	B	647	GLU	7.0
1	B	351	THR	7.0
1	B	437	VAL	7.0
1	A	79	MET	7.0
1	B	84	VAL	7.0
1	B	485	ASN	6.9
1	B	356	THR	6.9
2	H	205	TYR	6.9
1	A	163	GLU	6.9
1	B	282	LYS	6.9
2	G	120	THR	6.9
2	H	179	LYS	6.9
3	C	30	THR	6.9
1	B	517	ARG	6.9
1	A	226	GLN	6.9
1	A	482	ILE	6.9
1	A	751	GLU	6.9
1	A	111	THR	6.9
1	B	486	MET	6.9
1	A	648	LEU	6.9
2	G	108	GLY	6.9
1	A	581	SER	6.9
3	D	48	ASP	6.9
1	A	584	ARG	6.9
1	B	50	GLU	6.9
1	A	415	PHE	6.9
1	A	81	PRO	6.8
2	H	263	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	147	PHE	6.8
1	A	307	VAL	6.8
1	B	414	LYS	6.8
2	G	91	THR	6.8
1	A	334	HIS	6.8
1	B	177	ASN	6.8
2	H	264	PRO	6.8
1	A	141	MET	6.8
1	A	191	LEU	6.8
3	C	47	LEU	6.8
1	A	600	ASP	6.8
1	A	131	GLU	6.8
1	A	621	GLU	6.8
2	G	116	THR	6.8
1	A	684	MET	6.8
1	B	91	ALA	6.8
1	B	710	GLU	6.8
1	B	17	ASN	6.8
1	A	228	ALA	6.8
2	G	110	TYR	6.8
1	A	195	GLN	6.7
2	H	170	VAL	6.7
1	A	583	LYS	6.7
2	G	304	PHE	6.7
1	B	49	LYS	6.7
2	H	76	GLY	6.7
2	H	201	VAL	6.7
1	A	318	SER	6.7
1	A	728	ILE	6.7
2	H	157	ILE	6.7
3	C	61	LEU	6.7
1	A	549	PHE	6.7
2	H	111	LYS	6.7
2	G	214	GLY	6.7
2	H	191	ALA	6.7
1	B	507	VAL	6.7
2	H	394	TYR	6.7
1	A	465	GLU	6.7
1	A	524	GLY	6.7
1	A	119	LEU	6.7
1	A	458	VAL	6.7
1	B	599	TYR	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	436	THR	6.6
2	H	275	ILE	6.6
1	B	502	LEU	6.6
1	A	23	ALA	6.6
1	A	743	TYR	6.6
1	A	713	LYS	6.6
1	B	727	HIS	6.6
2	H	194	VAL	6.6
1	B	413	GLY	6.6
1	B	391	THR	6.6
1	B	706	GLU	6.6
1	A	117	ASN	6.6
1	A	245	LYS	6.6
1	A	437	VAL	6.6
2	H	359	TYR	6.6
2	H	253	ARG	6.6
2	H	138	GLN	6.6
1	A	588	ASN	6.6
1	A	770	GLU	6.6
2	G	226	ILE	6.6
1	A	73	SER	6.6
1	A	60	ASP	6.6
1	B	82	PHE	6.6
1	B	601	ASP	6.6
1	A	606	GLN	6.6
1	B	618	ILE	6.5
1	A	538	TYR	6.5
2	H	258	GLY	6.5
1	A	361	PHE	6.5
2	G	60	ASP	6.5
1	A	393	PRO	6.5
1	B	237	ALA	6.5
1	B	272	ALA	6.5
1	B	570	GLN	6.5
1	B	366	LYS	6.5
4	F	26	ARG	6.5
1	A	532	PRO	6.5
3	C	48	ASP	6.5
1	B	306	TYR	6.5
2	H	323	THR	6.5
1	A	629	ASN	6.5
2	H	58	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	338	GLU	6.5
2	G	75	LEU	6.5
1	B	745	GLN	6.5
1	A	486	MET	6.5
1	B	508	VAL	6.4
1	B	700	GLU	6.4
4	F	59	GLY	6.4
1	B	299	ALA	6.4
1	B	354	THR	6.4
1	B	409	ARG	6.4
3	D	51	PHE	6.4
1	B	665	TYR	6.4
1	B	270	GLU	6.4
4	E	36	GLY	6.4
1	A	644	PRO	6.4
4	F	52	THR	6.4
1	B	756	GLY	6.4
2	G	76	GLY	6.4
1	B	625	GLU	6.4
1	B	147	PHE	6.4
1	B	174	TYR	6.4
1	A	709	ARG	6.4
1	A	273	PHE	6.4
2	H	114	GLU	6.4
1	A	726	ASP	6.4
1	B	385	TYR	6.4
1	B	230	SER	6.4
1	B	221	LEU	6.4
1	B	677	PHE	6.4
1	A	177	ASN	6.4
4	F	34	GLY	6.4
1	A	706	GLU	6.4
1	B	640	ALA	6.4
2	G	175	ARG	6.4
2	G	286	SER	6.4
2	H	230	VAL	6.3
1	B	280	ASP	6.3
2	H	409	ASP	6.3
1	A	587	GLY	6.3
2	H	405	GLY	6.3
1	A	198	GLN	6.3
1	B	352	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	767	ILE	6.3
2	G	192	GLY	6.3
2	G	103	GLU	6.3
1	A	426	TYR	6.3
1	B	207	ASP	6.3
2	G	287	THR	6.3
1	B	701	GLU	6.3
1	B	525	ARG	6.3
1	B	398	VAL	6.3
1	B	362	ARG	6.3
1	A	135	SER	6.3
1	B	575	SER	6.3
2	H	227	ALA	6.3
1	A	439	VAL	6.3
1	A	568	PRO	6.3
1	A	650	GLU	6.3
2	G	199	ASN	6.3
2	G	255	LEU	6.3
1	A	475	GLY	6.2
1	A	756	GLY	6.2
4	F	45	GLY	6.2
1	A	774	PHE	6.2
1	A	508	VAL	6.2
1	B	67	ALA	6.2
1	A	180	LEU	6.2
2	G	203	GLN	6.2
1	A	109	THR	6.2
1	A	371	THR	6.2
1	A	165	ARG	6.2
1	A	572	LYS	6.2
1	B	680	GLU	6.2
2	H	349	GLY	6.2
2	G	242	ILE	6.2
1	B	333	LEU	6.2
1	A	309	GLU	6.2
1	B	329	TYR	6.2
1	A	254	ILE	6.2
1	B	339	ALA	6.2
1	B	452	LYS	6.2
2	H	69	ARG	6.2
1	A	326	GLY	6.2
1	A	138	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	79	MET	6.2
1	A	105	GLY	6.2
1	A	159	MET	6.2
1	A	719	ALA	6.2
1	B	125	HIS	6.2
4	E	62	PHE	6.2
1	B	619	ASP	6.2
1	B	416	LYS	6.2
1	B	396	ARG	6.1
2	G	186	SER	6.1
1	B	661	ILE	6.1
1	B	685	LEU	6.1
1	B	750	ARG	6.1
2	G	26	VAL	6.1
1	B	204	ALA	6.1
2	H	113	ASN	6.1
1	B	153	GLY	6.1
1	B	332	GLY	6.1
1	A	68	VAL	6.1
1	A	189	MET	6.1
1	B	520	ASN	6.1
1	A	670	ALA	6.1
2	H	178	GLU	6.1
1	A	89	GLY	6.1
1	A	297	HIS	6.1
1	A	771	VAL	6.1
2	G	191	ALA	6.1
1	B	771	VAL	6.1
1	B	13	LYS	6.1
1	A	567	THR	6.0
1	B	757	PHE	6.0
2	G	312	ASN	6.0
2	G	94	ILE	6.0
1	A	98	ALA	6.0
1	A	219	THR	6.0
1	B	506	ALA	6.0
2	G	268	ASN	6.0
2	G	300	ILE	6.0
2	H	252	GLY	6.0
1	B	670	ALA	6.0
2	G	384	LEU	6.0
2	H	242	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	83	LYS	6.0
1	B	61	LEU	6.0
3	C	43	TYR	6.0
2	G	251	VAL	6.0
1	A	263	GLU	6.0
1	B	83	LYS	6.0
1	B	245	LYS	6.0
1	A	754	MET	6.0
1	A	485	ASN	6.0
2	H	129	LEU	6.0
1	B	51	ARG	6.0
2	H	333	PRO	6.0
2	G	311	TYR	6.0
1	A	547	ARG	6.0
1	B	211	SER	6.0
1	B	320	THR	5.9
2	G	109	ARG	5.9
1	A	511	GLU	5.9
1	B	331	GLU	5.9
2	H	383	ILE	5.9
1	B	617	VAL	5.9
3	C	32	SER	5.9
2	G	171	TRP	5.9
2	G	380	LEU	5.9
1	A	590	PHE	5.9
2	G	342	LYS	5.9
2	G	208	VAL	5.9
1	B	37	SER	5.9
1	A	301	GLN	5.9
1	B	518	ILE	5.9
1	B	748	PRO	5.9
2	H	269	PRO	5.9
2	G	24	MET	5.9
2	H	171	TRP	5.9
1	A	53	GLU	5.9
1	A	184	TYR	5.9
1	B	163	GLU	5.9
1	B	250	TYR	5.9
1	A	396	ARG	5.9
1	A	384	ILE	5.9
2	G	381	ILE	5.9
1	A	387	MET	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	431	PRO	5.9
1	B	141	MET	5.9
1	A	734	LEU	5.9
1	B	729	ASP	5.9
1	B	383	ASN	5.9
1	A	55	GLY	5.9
1	A	181	GLY	5.9
2	G	165	GLY	5.9
2	G	394	TYR	5.9
1	A	412	GLU	5.9
1	B	425	ARG	5.9
1	A	720	VAL	5.9
1	A	483	ALA	5.9
1	B	134	ALA	5.9
2	H	73	PHE	5.8
2	H	116	THR	5.8
1	A	523	ARG	5.8
1	B	403	ARG	5.8
2	H	139	VAL	5.8
1	A	224	SER	5.8
2	H	270	ALA	5.8
2	G	28	TYR	5.8
2	G	86	MET	5.8
2	H	185	ALA	5.8
1	B	349	SER	5.8
1	A	358	GLN	5.8
1	A	137	ASP	5.8
1	A	429	GLY	5.8
1	B	694	THR	5.8
2	G	73	PHE	5.8
2	G	190	PHE	5.8
1	A	413	GLY	5.8
1	B	289	HIS	5.8
1	B	512	ARG	5.8
4	E	71	VAL	5.8
1	A	421	ASP	5.7
2	H	29	ARG	5.7
1	A	556	ALA	5.7
1	B	133	LEU	5.7
2	H	97	LEU	5.7
2	H	215	PRO	5.7
1	A	94	ASP	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	192	TYR	5.7
1	B	536	GLN	5.7
1	A	509	GLY	5.7
2	H	162	LEU	5.7
1	B	557	MET	5.7
1	B	178	ASN	5.7
1	B	40	ALA	5.7
1	B	489	ARG	5.7
4	E	72	ILE	5.7
1	B	321	GLY	5.7
1	B	35	ASN	5.7
1	B	566	SER	5.7
4	F	64	VAL	5.7
1	B	717	LEU	5.7
1	A	669	GLY	5.7
1	A	417	ALA	5.7
1	B	212	ILE	5.7
2	G	276	ILE	5.7
1	B	248	LYS	5.6
1	B	182	PHE	5.6
1	B	358	GLN	5.6
2	G	83	ALA	5.6
1	B	450	LYS	5.6
1	B	768	GLU	5.6
2	H	243	PRO	5.6
1	B	70	ARG	5.6
1	B	645	ARG	5.6
2	G	68	GLY	5.6
1	A	167	ALA	5.6
1	A	281	VAL	5.6
1	B	389	VAL	5.6
1	A	628	GLU	5.6
1	B	291	ASN	5.6
2	G	367	LEU	5.6
2	G	309	ILE	5.6
1	B	298	VAL	5.6
2	G	21	THR	5.6
2	H	159	VAL	5.6
1	A	116	LEU	5.6
2	G	30	LEU	5.6
1	A	760	PHE	5.6
1	B	692	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
2	H	140	SER	5.6
1	A	206	ILE	5.6
1	A	739	HIS	5.6
3	C	46	ILE	5.6
2	H	31	GLY	5.6
2	G	168	PHE	5.6
1	B	288	HIS	5.6
1	A	211	SER	5.6
1	B	88	GLY	5.6
1	B	527	GLY	5.6
1	B	85	GLN	5.6
1	B	728	ILE	5.6
1	B	712	GLU	5.6
1	A	126	VAL	5.5
1	B	293	ALA	5.5
1	B	140	GLN	5.5
2	G	378	ILE	5.5
1	B	63	VAL	5.5
1	A	522	LEU	5.5
2	H	164	ALA	5.5
4	E	51	LEU	5.5
1	A	110	SER	5.5
2	G	34	ILE	5.5
2	H	241	ARG	5.5
1	A	716	VAL	5.5
1	B	203	PHE	5.5
1	B	312	GLN	5.5
2	H	15	ARG	5.5
2	H	382	PRO	5.5
1	A	578	VAL	5.5
2	G	169	LEU	5.5
2	G	194	VAL	5.5
1	A	461	ALA	5.5
1	B	744	ALA	5.5
1	A	290	ILE	5.5
4	F	62	PHE	5.5
1	B	327	ARG	5.5
1	A	469	GLN	5.5
1	B	505	LEU	5.5
2	G	289	LEU	5.5
3	D	50	THR	5.5
1	A	440	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
2	G	9	PHE	5.5
2	H	402	ILE	5.5
1	A	515	SER	5.5
1	B	110	SER	5.5
2	G	254	GLN	5.5
2	H	182	GLY	5.5
1	A	703	PHE	5.5
1	B	9	PHE	5.5
1	B	473	GLU	5.5
2	H	261	THR	5.5
1	B	101	LYS	5.5
1	B	25	ASP	5.5
1	A	316	VAL	5.5
1	A	623	LEU	5.5
1	B	687	LEU	5.5
2	G	262	TYR	5.5
4	F	70	SER	5.5
1	B	392	ILE	5.5
1	B	202	HIS	5.5
2	G	23	LEU	5.4
2	H	75	LEU	5.4
1	A	729	ASP	5.4
2	G	179	LYS	5.4
1	A	344	GLU	5.4
1	B	387	MET	5.4
1	A	519	ASP	5.4
2	G	302	ASP	5.4
1	A	452	LYS	5.4
1	A	488	GLY	5.4
1	B	257	LYS	5.4
1	A	738	ILE	5.4
1	A	185	LEU	5.4
1	A	267	THR	5.4
1	B	311	GLY	5.4
2	H	143	GLY	5.4
3	D	34	ILE	5.4
1	A	542	GLU	5.4
1	A	641	ALA	5.4
1	A	742	ALA	5.4
2	G	266	LYS	5.4
2	G	372	ALA	5.4
2	H	61	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
2	H	222	ILE	5.4
1	A	317	ASP	5.4
4	F	9	PHE	5.4
1	B	87	MET	5.4
1	A	677	PHE	5.4
1	B	78	GLY	5.4
1	B	778	ALA	5.4
2	H	151	GLY	5.4
1	A	122	LYS	5.3
1	A	487	ALA	5.3
2	G	184	GLY	5.3
4	F	38	GLY	5.3
2	H	416	THR	5.3
4	F	44	VAL	5.3
1	B	363	MET	5.3
1	B	459	LEU	5.3
1	B	654	LEU	5.3
2	G	84	SER	5.3
2	H	228	ILE	5.3
2	H	267	ILE	5.3
1	B	183	ASP	5.3
2	G	176	ILE	5.3
2	H	304	PHE	5.3
1	A	722	SER	5.3
2	H	195	ALA	5.3
2	H	424	LYS	5.3
2	H	232	ILE	5.3
1	A	61	LEU	5.3
1	A	740	LEU	5.3
1	A	369	GLY	5.3
1	A	611	TYR	5.3
1	B	737	GLY	5.3
1	A	314	VAL	5.3
2	H	367	LEU	5.3
1	B	24	ASN	5.3
1	B	173	THR	5.2
2	G	419	ILE	5.2
1	A	356	THR	5.2
1	B	742	ALA	5.2
1	B	725	MET	5.2
1	B	254	ILE	5.2
1	B	345	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	322	ARG	5.2
1	A	42	LYS	5.2
1	A	360	TYR	5.2
2	G	78	MET	5.2
2	G	324	TYR	5.2
2	H	423	TYR	5.2
2	G	37	PRO	5.2
1	A	710	GLU	5.2
1	B	208	GLU	5.2
1	B	655	ASP	5.2
2	H	167	MET	5.2
2	G	327	THR	5.2
1	A	59	ASP	5.2
1	A	16	LEU	5.2
1	A	78	GLY	5.2
3	C	58	ILE	5.2
1	A	526	SER	5.2
1	A	337	ILE	5.2
1	B	774	PHE	5.2
2	G	369	PHE	5.2
2	G	370	PHE	5.2
1	B	567	THR	5.2
3	C	52	THR	5.2
2	H	12	LYS	5.2
3	C	28	LYS	5.2
1	B	446	SER	5.2
2	G	405	GLY	5.2
2	H	345	ALA	5.2
4	F	54	ALA	5.2
1	B	58	THR	5.1
1	A	108	LEU	5.1
1	A	127	VAL	5.1
1	B	180	LEU	5.1
4	E	8	LEU	5.1
1	B	769	ASP	5.1
2	G	359	TYR	5.1
1	B	304	VAL	5.1
1	B	683	GLU	5.1
1	B	590	PHE	5.1
2	G	36	ILE	5.1
1	A	492	ASP	5.1
1	A	160	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	143	LYS	5.1
4	E	70	SER	5.1
1	B	108	LEU	5.1
2	G	247	PRO	5.1
1	A	37	SER	5.1
1	B	662	ASN	5.1
2	H	266	LYS	5.1
1	B	538	TYR	5.1
1	B	137	ASP	5.1
2	G	303	MET	5.1
1	A	217	ALA	5.1
1	A	525	ARG	5.1
1	B	74	ARG	5.1
1	A	212	ILE	5.1
1	A	269	ALA	5.1
1	B	705	LYS	5.1
1	A	503	GLY	5.1
1	B	15	THR	5.1
1	A	113	PRO	5.1
1	B	152	VAL	5.1
1	B	292	GLN	5.1
1	A	618	ILE	5.1
1	A	293	ALA	5.0
1	B	188	ASN	5.0
2	H	307	GLY	5.0
1	B	264	GLU	5.0
1	B	370	MET	5.0
1	B	89	GLY	5.0
2	G	271	GLY	5.0
3	C	31	ILE	5.0
1	A	423	ALA	5.0
1	A	310	ASP	5.0
1	B	614	ARG	5.0
2	G	386	SER	5.0
2	G	390	ASN	5.0
2	H	198	PRO	5.0
1	A	97	ILE	5.0
1	A	143	LYS	5.0
2	G	209	LYS	5.0
2	H	364	ILE	5.0
4	E	17	ILE	5.0
2	H	57	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	265	GLY	5.0
2	H	184	GLY	5.0
1	B	519	ASP	5.0
4	E	28	ASP	5.0
1	A	434	VAL	5.0
1	B	773	LYS	5.0
1	A	466	ARG	5.0
2	G	379	ALA	5.0
1	B	602	VAL	5.0
1	A	731	MET	5.0
2	G	410	THR	5.0
2	G	146	VAL	5.0
1	A	541	MET	5.0
2	G	181	ILE	5.0
1	A	128	THR	5.0
1	A	322	ARG	5.0
1	B	754	MET	5.0
2	H	385	ILE	4.9
1	A	80	PHE	4.9
1	A	216	GLU	4.9
1	A	727	HIS	4.9
1	B	402	ASP	4.9
1	A	18	ARG	4.9
1	B	747	ASN	4.9
2	G	166	THR	4.9
1	A	602	VAL	4.9
1	B	648	LEU	4.9
2	G	319	ILE	4.9
2	G	185	ALA	4.9
1	A	95	GLY	4.9
1	A	424	GLN	4.9
2	G	144	ILE	4.9
2	H	16	GLN	4.9
1	B	334	HIS	4.9
3	D	37	SER	4.9
1	A	775	VAL	4.9
2	H	149	ASN	4.9
1	A	388	GLN	4.9
1	B	552	GLU	4.9
2	H	341	HIS	4.9
1	A	390	VAL	4.9
1	A	399	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	488	GLY	4.9
1	B	659	ASP	4.9
2	G	245	GLN	4.9
1	A	474	ALA	4.9
1	B	765	GLU	4.9
2	H	371	GLY	4.9
3	C	34	ILE	4.9
1	A	394	THR	4.9
2	H	272	VAL	4.9
1	A	239	ALA	4.8
1	A	778	ALA	4.8
1	A	88	GLY	4.8
1	B	702	GLN	4.8
1	B	164	LYS	4.8
1	A	516	ARG	4.8
1	B	500	LYS	4.8
1	B	743	TYR	4.8
2	G	246	TYR	4.8
3	C	56	SER	4.8
2	H	247	PRO	4.8
1	A	96	ASN	4.8
4	E	57	TRP	4.8
1	A	545	LEU	4.8
2	H	357	VAL	4.8
1	B	46	ILE	4.8
1	B	149	GLY	4.8
1	A	29	ILE	4.8
2	G	284	ILE	4.8
2	H	392	PRO	4.8
1	B	28	ALA	4.8
1	B	210	ASP	4.8
1	A	271	LYS	4.8
2	H	26	VAL	4.8
1	A	471	ILE	4.8
4	E	50	ILE	4.8
4	F	41	ILE	4.8
2	H	325	PHE	4.8
2	G	317	THR	4.8
2	G	294	ASN	4.8
1	B	526	SER	4.7
1	A	432	VAL	4.7
1	B	465	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
2	H	363	ILE	4.7
2	G	362	ARG	4.7
1	B	126	VAL	4.7
2	H	303	MET	4.7
1	B	410	THR	4.7
2	G	269	PRO	4.7
1	B	558	LEU	4.7
1	B	724	TRP	4.7
1	B	139	GLU	4.7
2	H	104	GLU	4.7
1	A	425	ARG	4.7
1	A	645	ARG	4.7
1	B	516	ARG	4.7
1	A	761	GLU	4.7
1	A	17	ASN	4.7
3	C	62	ARG	4.7
1	A	99	GLU	4.7
1	A	262	THR	4.7
2	G	325	PHE	4.7
1	A	283	HIS	4.7
1	A	256	THR	4.7
2	G	29	ARG	4.7
2	G	235	VAL	4.6
1	B	189	MET	4.6
1	B	206	ILE	4.6
1	A	730	ALA	4.6
1	A	243	THR	4.6
1	A	749	LEU	4.6
2	H	413	GLN	4.6
1	B	14	ARG	4.6
1	B	620	SER	4.6
1	B	60	ASP	4.6
1	B	172	ILE	4.6
2	H	192	GLY	4.6
1	B	607	ARG	4.6
1	A	398	VAL	4.6
1	A	585	VAL	4.6
1	A	101	LYS	4.6
1	A	675	ASP	4.6
2	G	422	LYS	4.6
2	G	265	ILE	4.6
2	H	285	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	21	LYS	4.6
1	B	263	GLU	4.6
2	G	253	ARG	4.6
1	A	304	VAL	4.6
1	A	638	ALA	4.6
2	G	402	ILE	4.6
2	H	403	VAL	4.6
1	A	121	GLY	4.6
2	G	160	LEU	4.6
2	H	20	PHE	4.6
1	A	146	GLU	4.6
4	E	49	THR	4.6
1	B	69	VAL	4.6
1	B	185	LEU	4.6
4	E	16	LEU	4.6
1	B	47	GLU	4.6
2	G	231	GLY	4.5
2	G	248	GLY	4.5
1	B	720	VAL	4.5
2	G	314	LEU	4.5
2	H	86	MET	4.5
4	F	55	THR	4.5
2	H	108	GLY	4.5
1	A	235	VAL	4.5
1	B	201	LEU	4.5
2	G	97	LEU	4.5
2	H	63	SER	4.5
2	H	207	LYS	4.5
1	A	303	ASP	4.5
2	H	120	THR	4.5
1	A	755	GLU	4.5
1	A	205	VAL	4.5
2	G	92	VAL	4.5
1	B	360	TYR	4.5
1	B	577	ALA	4.5
2	G	354	GLN	4.5
1	A	323	LEU	4.5
2	G	121	LEU	4.5
1	A	595	GLN	4.5
1	A	199	ARG	4.5
1	B	703	PHE	4.5
1	B	158	SER	4.5

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Mol	Chain	Res	Type	RSRZ
4	E	19	SER	4.5
1	A	133	LEU	4.5
1	A	333	LEU	4.5
2	H	356	THR	4.5
1	B	315	ILE	4.5
2	G	228	ILE	4.5
1	A	759	MET	4.5
2	H	400	ALA	4.5
2	H	65	GLY	4.5
2	H	11	LEU	4.4
1	A	391	THR	4.4
1	A	692	ILE	4.4
2	G	273	ILE	4.4
1	A	763	MET	4.4
1	A	520	ASN	4.4
1	B	513	HIS	4.4
1	B	761	GLU	4.4
2	G	227	ALA	4.4
2	G	361	GLU	4.4
2	H	83	ALA	4.4
1	B	480	VAL	4.4
4	F	60	ALA	4.4
1	A	451	ASN	4.4
2	H	127	GLN	4.4
4	F	47	VAL	4.4
2	H	158	THR	4.4
4	E	55	THR	4.4
1	A	115	TYR	4.4
1	A	505	LEU	4.4
1	B	275	ILE	4.4
1	B	676	ILE	4.4
2	H	377	VAL	4.4
1	B	226	GLN	4.4
2	H	250	GLN	4.4
1	A	405	ASP	4.4
1	B	559	ASP	4.4
3	C	50	THR	4.4
1	B	95	GLY	4.4
1	B	97	ILE	4.4
1	B	390	VAL	4.4
2	G	193	ILE	4.4
2	H	229	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
3	C	37	SER	4.4
1	A	414	LYS	4.4
2	H	314	LEU	4.4
4	F	58	LEU	4.4
1	B	514	GLU	4.4
2	H	265	ILE	4.4
2	H	338	GLU	4.4
2	H	427	VAL	4.4
1	B	330	SER	4.4
1	A	718	ARG	4.4
1	A	546	MET	4.4
1	B	406	LEU	4.4
1	B	461	ALA	4.3
2	G	170	VAL	4.3
2	G	178	GLU	4.3
1	A	255	LYS	4.3
1	A	622	ASN	4.3
1	A	400	ARG	4.3
1	A	735	ARG	4.3
2	H	415	GLU	4.3
1	A	327	ARG	4.3
2	G	403	VAL	4.3
4	E	30	GLY	4.3
4	E	21	LEU	4.3
1	B	587	GLY	4.3
2	G	18	PHE	4.3
2	H	369	PHE	4.3
1	B	138	ALA	4.3
2	G	250	GLN	4.3
2	H	59	TYR	4.3
1	A	324	MET	4.3
1	A	39	ASP	4.3
1	B	610	ILE	4.3
2	G	375	LEU	4.3
1	B	255	LYS	4.3
1	A	512	ARG	4.3
2	H	305	GLN	4.3
2	H	393	PHE	4.3
2	G	142	LYS	4.3
4	E	35	GLY	4.3
1	A	463	ASN	4.3
1	A	136	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	167	ALA	4.2
1	A	240	PHE	4.2
1	A	106	LYS	4.2
2	G	35	PRO	4.2
1	B	682	ASP	4.2
1	B	26	ILE	4.2
2	H	208	VAL	4.2
1	B	611	TYR	4.2
2	H	245	GLN	4.2
1	A	732	ASP	4.2
1	A	489	ARG	4.2
1	B	400	ARG	4.2
2	G	189	ILE	4.2
2	H	181	ILE	4.2
1	B	68	VAL	4.2
4	F	57	TRP	4.2
1	B	318	SER	4.2
1	B	77	THR	4.2
2	H	336	LEU	4.2
2	G	64	GLY	4.2
1	B	441	THR	4.2
1	B	767	ILE	4.2
2	H	19	ILE	4.2
1	A	773	LYS	4.2
1	B	723	LYS	4.2
1	A	478	GLY	4.2
1	A	599	TYR	4.2
1	B	44	LYS	4.2
2	G	424	LYS	4.2
3	C	33	VAL	4.2
1	A	22	ILE	4.1
2	G	297	ILE	4.1
2	G	363	ILE	4.1
1	B	604	ARG	4.1
2	G	22	LEU	4.1
1	A	63	VAL	4.1
1	A	193	LYS	4.1
1	B	8	MET	4.1
1	A	441	THR	4.1
2	G	229	ILE	4.1
3	C	55	ILE	4.1
1	A	21	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
2	G	136	ARG	4.1
1	B	422	VAL	4.1
2	H	74	ALA	4.1
2	H	169	LEU	4.1
1	B	584	ARG	4.1
2	H	92	VAL	4.1
2	H	235	VAL	4.1
1	A	406	LEU	4.1
4	E	66	ALA	4.1
4	F	39	GLN	4.1
2	H	94	ILE	4.1
1	A	619	ASP	4.1
1	B	574	VAL	4.1
2	G	406	VAL	4.1
2	H	33	HIS	4.1
1	B	521	GLN	4.1
1	A	286	LEU	4.1
2	H	368	ILE	4.1
1	A	422	VAL	4.1
1	A	721	ASP	4.1
1	A	204	ALA	4.1
1	A	220	PRO	4.1
1	B	170	ALA	4.1
1	B	568	PRO	4.1
2	H	70	LEU	4.1
1	A	26	ILE	4.1
1	A	676	ILE	4.1
1	B	580	SER	4.1
3	D	28	LYS	4.1
1	B	30	ARG	4.1
1	B	109	THR	4.1
1	A	649	PRO	4.0
1	A	748	PRO	4.0
2	G	328	ALA	4.0
1	A	190	VAL	4.0
2	G	82	SER	4.0
2	H	231	GLY	4.0
2	G	345	ALA	4.0
1	A	7	LYS	4.0
1	B	576	ARG	4.0
2	H	196	ASN	4.0
2	H	64	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
2	G	156	LEU	4.0
1	A	683	GLU	4.0
1	B	222	ILE	4.0
1	B	421	ASP	4.0
1	B	624	ARG	4.0
1	A	114	VAL	4.0
1	A	561	PHE	4.0
1	B	615	PHE	4.0
2	G	137	GLY	4.0
2	G	296	PHE	4.0
1	B	340	LYS	4.0
1	B	146	GLU	4.0
2	G	366	ARG	4.0
2	G	123	VAL	4.0
1	B	41	LEU	4.0
2	H	121	LEU	4.0
1	A	626	ILE	4.0
2	G	295	PRO	4.0
2	H	88	GLN	4.0
2	H	384	LEU	4.0
1	A	242	ARG	4.0
2	H	233	VAL	4.0
2	H	404	VAL	4.0
1	A	435	GLY	4.0
1	A	479	ALA	4.0
2	H	175	ARG	4.0
1	B	522	LEU	3.9
2	H	110	TYR	3.9
1	A	560	ARG	3.9
2	G	334	VAL	3.9
1	A	319	PHE	3.9
1	A	504	GLY	3.9
1	B	471	ILE	3.9
2	G	14	LEU	3.9
1	A	164	LYS	3.9
2	G	155	ILE	3.9
4	F	15	VAL	3.9
1	A	711	PHE	3.9
1	A	724	TRP	3.9
4	E	56	TYR	3.9
1	A	551	ALA	3.9
2	G	418	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	308	ALA	3.9
3	D	33	VAL	3.9
1	B	766	SER	3.9
1	A	378	GLU	3.9
1	A	134	ALA	3.9
2	G	278	ALA	3.9
1	B	554	THR	3.9
3	C	42	VAL	3.9
2	G	333	PRO	3.9
1	A	112	LEU	3.9
1	A	343	LEU	3.9
1	A	636	GLU	3.9
1	B	16	LEU	3.9
4	F	51	LEU	3.9
1	B	582	GLN	3.8
1	B	94	ASP	3.8
2	H	112	ILE	3.8
2	H	271	GLY	3.8
3	D	31	ILE	3.8
4	E	59	GLY	3.8
1	B	186	ARG	3.8
2	G	197	PHE	3.8
2	H	321	PHE	3.8
2	H	165	GLY	3.8
2	H	60	ASP	3.8
1	B	115	TYR	3.8
1	A	462	LYS	3.8
2	G	93	ALA	3.8
2	H	354	GLN	3.8
2	H	330	LEU	3.8
4	E	58	LEU	3.8
1	A	708	MET	3.8
1	A	46	ILE	3.8
1	A	717	LEU	3.8
1	B	184	TYR	3.8
1	A	24	ASN	3.8
1	A	158	SER	3.8
1	A	777	LYS	3.8
2	H	80	TYR	3.8
1	B	616	GLU	3.8
1	B	666	LEU	3.8
1	A	332	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	446	SER	3.8
1	A	241	VAL	3.8
1	A	499	VAL	3.8
1	B	145	PHE	3.8
1	A	518	ILE	3.8
1	B	223	ILE	3.8
1	B	119	LEU	3.8
1	B	365	GLU	3.8
2	G	119	LEU	3.8
1	A	302	LYS	3.7
1	A	477	LYS	3.7
1	A	537	PHE	3.7
1	B	73	SER	3.7
2	G	88	GLN	3.7
1	A	564	ASP	3.7
1	A	682	ASP	3.7
2	H	334	VAL	3.7
1	B	442	SER	3.7
1	A	596	LEU	3.7
1	A	565	ASP	3.7
1	B	523	ARG	3.7
1	A	459	LEU	3.7
1	B	631	ILE	3.7
1	B	772	ALA	3.7
1	A	593	ARG	3.7
1	A	331	GLU	3.7
2	H	135	ILE	3.7
1	B	553	ARG	3.7
1	A	34	GLU	3.7
1	A	698	GLU	3.7
1	B	150	LEU	3.7
2	H	262	TYR	3.7
1	A	74	ARG	3.7
2	G	87	MET	3.7
1	B	99	GLU	3.7
1	B	348	GLU	3.7
2	H	373	LEU	3.7
1	B	419	ALA	3.7
2	G	320	VAL	3.7
3	D	56	SER	3.7
3	D	30	THR	3.7
1	B	542	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	G	275	ILE	3.7
1	A	416	LYS	3.7
2	G	234	TYR	3.7
2	H	77	VAL	3.6
2	H	186	SER	3.6
1	B	92	LEU	3.6
1	B	251	THR	3.6
2	G	33	HIS	3.6
1	A	772	ALA	3.6
1	B	38	ASP	3.6
1	A	266	MET	3.6
2	H	119	LEU	3.6
1	A	510	THR	3.6
1	B	481	THR	3.6
2	G	188	ILE	3.6
1	A	194	GLU	3.6
1	A	640	ALA	3.6
1	A	613	GLN	3.6
1	A	215	ASP	3.6
1	B	449	LEU	3.6
1	A	306	TYR	3.6
1	B	751	GLU	3.6
1	A	609	VAL	3.6
1	B	18	ARG	3.6
1	B	316	VAL	3.6
1	B	144	ILE	3.6
2	G	215	PRO	3.6
2	G	285	PRO	3.6
1	B	663	THR	3.6
1	B	418	VAL	3.6
4	F	61	LEU	3.6
1	B	151	THR	3.6
1	B	227	ALA	3.6
2	G	20	PHE	3.6
2	G	216	LEU	3.6
3	D	44	LEU	3.6
4	F	21	LEU	3.6
2	G	392	PRO	3.6
2	G	310	PHE	3.6
1	A	348	GLU	3.6
1	A	768	GLU	3.6
2	H	327	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	610	ILE	3.6
2	G	353	GLY	3.6
1	A	210	ASP	3.5
4	E	40	SER	3.5
1	A	433	LEU	3.5
2	G	401	LEU	3.5
1	B	730	ALA	3.5
2	G	211	GLY	3.5
1	A	604	ARG	3.5
4	E	15	VAL	3.5
2	G	232	ILE	3.5
1	A	634	SER	3.5
1	B	344	GLU	3.5
1	A	321	GLY	3.5
4	E	20	THR	3.5
1	B	384	ILE	3.5
2	H	309	ILE	3.5
1	B	660	LEU	3.5
2	H	14	LEU	3.5
1	A	367	LEU	3.5
1	A	550	GLY	3.5
1	A	282	LYS	3.5
1	B	487	ALA	3.5
2	H	223	ALA	3.5
1	B	294	LEU	3.5
1	A	690	ASP	3.5
1	A	418	VAL	3.5
1	B	338	GLU	3.5
1	B	722	SER	3.5
1	B	301	GLN	3.5
1	B	376	THR	3.5
1	A	407	ILE	3.5
1	B	515	SER	3.4
1	B	595	GLN	3.4
1	A	339	ALA	3.4
1	A	213	LEU	3.4
1	A	289	HIS	3.4
1	B	462	LYS	3.4
1	A	27	ASP	3.4
1	B	543	ASP	3.4
2	H	335	GLU	3.4
2	H	378	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	140	GLN	3.4
1	A	221	LEU	3.4
2	G	129	LEU	3.4
2	H	360	LEU	3.4
1	A	594	LYS	3.4
2	G	404	VAL	3.4
1	B	440	GLU	3.4
1	A	419	ALA	3.4
1	A	36	LEU	3.4
1	A	200	PRO	3.4
4	E	54	ALA	3.4
1	A	582	GLN	3.4
3	C	49	LEU	3.4
1	A	576	ARG	3.4
2	G	12	LYS	3.4
2	H	79	PRO	3.4
1	A	45	THR	3.4
3	C	35	ILE	3.4
1	A	352	LEU	3.4
1	A	513	HIS	3.4
1	A	579	GLU	3.4
1	A	397	PRO	3.4
2	H	17	LYS	3.4
2	H	166	THR	3.4
2	G	344	GLY	3.4
1	A	448	LEU	3.4
4	E	65	LEU	3.4
1	A	380	GLU	3.4
1	B	11	PRO	3.4
2	G	417	TYR	3.4
1	A	274	GLY	3.4
1	A	498	GLY	3.4
1	B	626	ILE	3.4
1	B	764	ILE	3.4
3	D	61	LEU	3.4
1	A	49	LYS	3.3
1	B	276	ASP	3.3
1	A	148	LEU	3.3
1	A	58	THR	3.3
2	G	399	THR	3.3
2	H	337	ALA	3.3
1	B	295	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	G	306	PRO	3.3
1	B	313	VAL	3.3
4	F	17	ILE	3.3
2	G	343	ALA	3.3
2	H	411	PHE	3.3
2	G	377	VAL	3.3
4	E	11	ILE	3.3
4	F	65	LEU	3.3
2	H	82	SER	3.3
2	H	310	PHE	3.3
1	B	283	HIS	3.3
2	G	145	PRO	3.3
1	B	267	THR	3.3
2	G	113	ASN	3.3
1	A	392	ILE	3.3
1	A	64	GLU	3.3
1	B	420	GLU	3.3
1	B	342	GLY	3.3
2	G	308	ALA	3.3
2	H	313	PHE	3.3
1	B	433	LEU	3.3
1	B	671	LEU	3.3
2	G	283	LEU	3.3
2	H	27	ILE	3.3
1	A	225	GLY	3.3
1	B	90	VAL	3.3
1	A	776	MET	3.3
2	H	339	ASN	3.2
1	A	577	ALA	3.2
1	A	750	ARG	3.2
2	H	93	ALA	3.2
1	B	541	MET	3.2
1	B	10	ASP	3.2
1	A	15	THR	3.2
1	A	695	LYS	3.2
1	A	342	GLY	3.2
1	B	504	GLY	3.2
1	A	272	ALA	3.2
2	G	224	LEU	3.2
4	F	71	VAL	3.2
4	F	50	ILE	3.2
1	B	168	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	53	LYS	3.2
1	B	464	HIS	3.2
2	G	71	THR	3.2
2	G	236	GLN	3.2
2	H	412	ARG	3.2
2	H	328	ALA	3.2
1	A	681	PRO	3.2
1	B	326	GLY	3.2
3	C	41	GLY	3.2
2	H	62	PHE	3.2
2	H	163	VAL	3.2
1	A	746	THR	3.2
1	B	12	THR	3.2
1	A	521	GLN	3.2
1	A	747	ASN	3.2
2	H	225	ILE	3.2
2	H	278	ALA	3.2
1	B	42	LYS	3.2
2	G	277	PHE	3.2
1	A	741	ARG	3.2
2	H	362	ARG	3.2
1	A	207	ASP	3.2
1	A	377	GLU	3.2
1	B	128	THR	3.2
1	B	693	ILE	3.2
3	D	29	ALA	3.2
1	A	457	GLN	3.2
2	H	312	ASN	3.2
2	H	324	TYR	3.2
1	A	470	ILE	3.2
2	G	225	ILE	3.2
4	F	23	GLN	3.1
2	G	332	ASN	3.1
2	H	418	LEU	3.1
2	H	123	VAL	3.1
2	G	39	ILE	3.1
1	A	287	ASN	3.1
1	A	725	MET	3.1
1	B	62	LEU	3.1
2	H	376	SER	3.1
2	H	408	LEU	3.1
2	G	122	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	229	LYS	3.1
1	A	366	LYS	3.1
2	H	101	ALA	3.1
2	G	330	LEU	3.1
1	B	377	GLU	3.1
2	H	236	GLN	3.1
3	D	62	ARG	3.1
2	H	87	MET	3.1
2	G	415	GLU	3.1
2	H	56	PHE	3.1
4	E	9	PHE	3.1
2	H	406	VAL	3.1
2	G	364	ILE	3.1
1	B	656	GLY	3.1
2	H	398	THR	3.1
3	C	59	LEU	3.1
1	B	381	PHE	3.1
1	B	711	PHE	3.1
1	B	627	VAL	3.1
4	E	27	GLY	3.0
2	G	174	ASP	3.0
2	G	217	THR	3.0
1	A	28	ALA	3.0
1	A	237	ALA	3.0
3	C	39	ALA	3.0
1	B	357	PHE	3.0
1	A	630	MET	3.0
1	B	763	MET	3.0
2	G	19	ILE	3.0
1	B	154	LEU	3.0
3	D	57	PHE	3.0
1	A	383	ASN	3.0
2	G	230	VAL	3.0
2	G	135	ILE	3.0
1	A	766	SER	3.0
1	B	262	THR	3.0
1	B	22	ILE	3.0
2	H	224	LEU	3.0
4	E	63	LEU	3.0
2	H	10	GLU	3.0
1	B	537	PHE	3.0
1	A	298	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	209	VAL	3.0
1	A	573	MET	3.0
3	D	41	GLY	3.0
4	E	25	GLY	3.0
2	G	10	GLU	3.0
1	B	474	ALA	3.0
1	B	308	VAL	3.0
4	E	14	VAL	3.0
1	B	59	ASP	3.0
2	G	398	THR	3.0
2	H	410	THR	3.0
1	B	213	LEU	3.0
2	G	17	LYS	3.0
1	B	29	ILE	3.0
1	B	367	LEU	3.0
1	B	224	SER	3.0
1	A	404	PRO	3.0
4	F	53	LYS	3.0
1	A	552	GLU	3.0
2	G	61	ILE	2.9
2	H	366	ARG	3.0
2	G	281	LEU	2.9
2	H	37	PRO	2.9
1	A	188	ASN	2.9
1	A	374	ALA	2.9
1	A	574	VAL	2.9
1	A	603	LEU	2.9
1	A	715	ILE	2.9
1	A	183	ASP	2.9
1	A	517	ARG	2.9
1	B	307	VAL	2.9
4	F	13	ALA	2.9
1	B	460	ASN	2.9
2	G	187	LEU	2.9
4	F	18	ILE	2.9
1	A	494	LYS	2.9
1	A	93	HIS	2.9
1	A	382	ARG	2.9
2	H	34	ILE	2.9
1	B	284	VAL	2.9
1	B	592	SER	2.9
1	B	638	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	124	ALA	2.9
1	A	350	MET	2.9
2	H	144	ILE	2.9
2	H	414	ILE	2.9
1	B	608	GLU	2.9
1	B	463	ASN	2.9
1	B	7	LYS	2.9
3	C	44	LEU	2.9
2	G	400	ALA	2.9
4	E	26	ARG	2.9
1	B	613	GLN	2.9
2	G	56	PHE	2.9
1	B	470	ILE	2.9
1	A	91	ALA	2.9
1	A	758	ALA	2.9
1	A	12	THR	2.9
2	H	18	PHE	2.8
1	A	214	ILE	2.8
1	B	499	VAL	2.8
1	B	603	LEU	2.8
1	B	114	VAL	2.8
2	H	417	TYR	2.8
2	G	79	PRO	2.8
2	G	207	LYS	2.8
1	B	112	LEU	2.8
1	A	381	PHE	2.8
1	A	691	ARG	2.8
2	G	412	ARG	2.8
2	H	251	VAL	2.8
1	B	776	MET	2.8
1	B	736	GLN	2.8
1	B	96	ASN	2.8
2	H	281	LEU	2.8
1	B	241	VAL	2.8
4	E	12	ILE	2.8
1	A	330	SER	2.8
1	B	36	LEU	2.8
1	B	323	LEU	2.8
2	H	216	LEU	2.8
4	E	18	ILE	2.8
1	A	443	GLU	2.8
1	B	113	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	G	282	LEU	2.8
2	H	153	SER	2.8
2	H	348	PRO	2.8
1	B	439	VAL	2.7
2	G	157	ILE	2.7
1	B	274	GLY	2.7
2	H	358	LYS	2.7
2	H	13	GLU	2.7
3	C	51	PHE	2.7
1	A	569	ILE	2.7
2	H	319	ILE	2.7
1	B	596	LEU	2.7
2	G	70	LEU	2.7
4	F	56	TYR	2.7
2	H	35	PRO	2.7
1	A	25	ASP	2.7
4	E	47	VAL	2.7
1	A	92	LEU	2.7
1	B	116	LEU	2.7
1	A	47	GLU	2.7
1	A	544	GLU	2.7
2	H	176	ILE	2.7
1	A	699	LYS	2.7
2	G	280	ALA	2.7
2	H	257	ALA	2.7
1	B	273	PHE	2.7
2	G	413	GLN	2.7
1	B	494	LYS	2.7
2	H	32	SER	2.7
4	F	66	ALA	2.7
1	A	87	MET	2.7
1	A	597	LEU	2.7
1	A	635	LEU	2.7
2	H	23	LEU	2.7
2	G	396	GLY	2.7
2	H	248	GLY	2.7
2	G	85	ILE	2.7
1	B	578	VAL	2.7
2	G	220	LEU	2.7
1	B	475	GLY	2.7
4	F	14	VAL	2.6
2	H	78	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	623	LEU	2.6
1	B	496	GLY	2.6
1	A	209	VAL	2.6
1	A	50	GLU	2.6
1	A	312	GLN	2.6
1	B	443	GLU	2.6
2	G	32	SER	2.6
2	G	421	LYS	2.6
1	A	559	ASP	2.6
3	D	59	LEU	2.6
1	A	686	GLU	2.6
1	A	601	ASP	2.6
2	H	370	PHE	2.6
4	F	24	LYS	2.6
2	G	57	ALA	2.6
1	B	555	MET	2.6
2	H	145	PRO	2.6
1	B	66	PHE	2.6
1	A	340	LYS	2.6
1	A	562	GLY	2.6
1	A	723	LYS	2.6
2	G	16	GLN	2.6
1	B	287	ASN	2.6
2	G	267	ILE	2.6
1	A	90	VAL	2.6
1	B	286	LEU	2.6
2	G	313	PHE	2.6
2	G	221	ILE	2.6
1	A	370	MET	2.6
2	H	28	TYR	2.6
2	H	85	ILE	2.5
2	H	187	LEU	2.5
1	A	14	ARG	2.5
1	A	208	GLU	2.5
1	A	120	THR	2.5
1	A	311	GLY	2.5
1	A	139	GLU	2.5
1	A	557	MET	2.5
2	H	361	GLU	2.5
2	G	326	TYR	2.5
1	B	341	GLU	2.5
2	H	156	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	159	VAL	2.5
2	G	249	ARG	2.5
1	B	194	GLU	2.5
1	A	450	LYS	2.5
1	A	203	PHE	2.5
4	F	72	ILE	2.5
2	H	329	VAL	2.5
4	F	10	VAL	2.5
2	G	38	GLY	2.5
2	H	177	THR	2.5
1	A	420	GLU	2.5
4	F	22	LEU	2.5
2	H	407	ALA	2.5
1	B	20	GLU	2.5
2	G	385	ILE	2.5
1	B	127	VAL	2.5
1	A	86	LEU	2.4
1	B	111	THR	2.4
1	B	240	PHE	2.4
3	C	36	PHE	2.4
1	B	290	ILE	2.4
1	B	733	GLN	2.4
1	B	317	ASP	2.4
1	B	657	LEU	2.4
1	A	365	GLU	2.4
3	D	42	VAL	2.4
1	A	445	ILE	2.4
1	A	364	TYR	2.4
3	D	40	ILE	2.4
1	B	755	GLU	2.4
2	H	100	LEU	2.4
1	B	19	TYR	2.4
1	A	186	ARG	2.4
1	B	34	GLU	2.4
1	B	447	LYS	2.4
4	E	22	LEU	2.4
2	H	397	GLY	2.4
1	A	9	PHE	2.4
2	G	346	PHE	2.4
1	B	593	ARG	2.4
4	E	53	LYS	2.4
1	B	681	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	G	200	ALA	2.3
2	G	149	ASN	2.3
1	B	285	ALA	2.3
3	D	58	ILE	2.3
2	G	360	LEU	2.3
2	H	326	TYR	2.3
1	A	288	HIS	2.3
1	B	72	ALA	2.3
1	B	246	ALA	2.3
2	H	237	GLU	2.3
1	A	403	ARG	2.3
1	B	695	LYS	2.3
2	H	239	GLU	2.3
1	B	190	VAL	2.3
2	H	117	LYS	2.3
1	A	376	THR	2.3
1	B	411	MET	2.3
2	G	112	ILE	2.3
2	H	306	PRO	2.3
2	H	391	ILE	2.3
2	H	38	GLY	2.3
1	A	627	VAL	2.3
1	A	182	PHE	2.3
2	G	81	ILE	2.3
1	A	202	HIS	2.3
2	H	84	SER	2.3
1	A	56	ALA	2.3
1	A	227	ALA	2.3
2	H	343	ALA	2.3
1	A	745	GLN	2.3
2	G	152	ILE	2.2
2	H	95	PRO	2.2
1	B	98	ALA	2.2
2	H	283	LEU	2.2
1	A	284	VAL	2.2
2	G	143	GLY	2.2
1	B	187	ASP	2.2
1	A	222	ILE	2.2
1	B	361	PHE	2.2
2	H	244	ILE	2.2
2	G	307	GLY	2.2
1	B	731	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	191	LEU	2.2
2	G	90	LEU	2.2
2	H	91	THR	2.2
2	H	189	ILE	2.2
3	C	57	PHE	2.2
4	E	42	PHE	2.2
3	D	38	LEU	2.2
2	G	233	VAL	2.2
2	G	11	LEU	2.2
1	A	10	ASP	2.2
1	A	187	ASP	2.2
1	B	269	ALA	2.2
2	H	199	ASN	2.2
1	A	145	PHE	2.2
1	A	687	LEU	2.2
1	B	777	LYS	2.2
1	B	634	SER	2.2
2	G	279	GLN	2.2
3	D	43	TYR	2.2
1	A	637	ARG	2.2
1	B	417	ALA	2.1
1	B	214	ILE	2.1
3	C	40	ILE	2.1
1	A	555	MET	2.1
1	B	225	GLY	2.1
2	G	256	TYR	2.1
2	H	279	GLN	2.1
1	B	378	GLU	2.1
2	G	13	GLU	2.1
2	H	332	ASN	2.1
1	A	612	LYS	2.1
1	B	698	GLU	2.1
1	A	62	LEU	2.1
1	B	148	LEU	2.1
2	G	336	LEU	2.1
2	G	408	LEU	2.1
1	B	117	ASN	2.1
2	H	311	TYR	2.0
1	B	445	ILE	2.0
1	B	760	PHE	2.0
2	H	218	LEU	2.0
2	G	411	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	G	65	GLY	2.0
1	B	242	ARG	2.0
1	B	633	SER	2.0
2	H	396	GLY	2.0
1	B	193	LYS	2.0
2	G	177	THR	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.