



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:57 AM GMT

PDB ID : 2VE8
Title : Xray structure of FtsK gamma domain (P. aeruginosa)
Authors : Lowe, J.; Allen, M.A.; Sherratt, D.J.
Deposited on : 2007-10-17
Resolution : 1.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

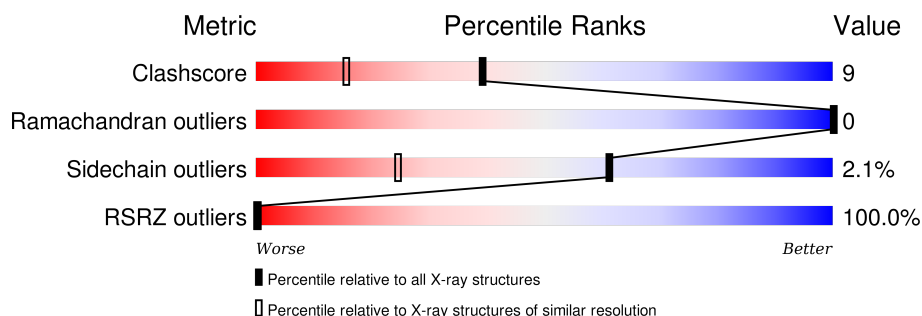
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1295 (1.40-1.40)
Ramachandran outliers	100387	1259 (1.40-1.40)
Sidechain outliers	100360	1258 (1.40-1.40)
RSRZ outliers	91569	1198 (1.40-1.40)

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

Mol	Chain	Length	Quality of chain
1	A	73	<div> <div>92%</div> <div> <div>77%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	73	<div> <div>89%</div> <div> <div>74%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	73	<div> <div>86%</div> <div> <div>71%</div> <div>10%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	73	<div> <div>93%</div> <div> <div>81%</div> <div>8%</div> <div>•</div> <div>7%</div> </div> </div>
1	E	73	<div> <div>92%</div> <div> <div>73%</div> <div>16%</div> <div>•</div> <div>8%</div> </div> </div>
1	F	73	<div> <div>90%</div> <div> <div>73%</div> <div>15%</div> <div>•</div> <div>10%</div> </div> </div>
1	G	73	<div> <div>84%</div> <div> <div>64%</div> <div>15%</div> <div>•</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	H	73	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>86%68%12%5%14%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4633 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 DNA TRANSLOCASE FTSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	S	0	0	0
			520	318	97	101	4			
1	B	65	Total	C	N	O	S	0	0	0
			500	308	92	96	4			
1	C	63	Total	C	N	O	S	0	0	1
			477	295	89	89	4			
1	D	68	Total	C	N	O	S	0	0	0
			526	321	98	103	4			
1	E	67	Total	C	N	O	S	0	0	1
			507	311	94	98	4			
1	F	66	Total	C	N	O	S	0	0	1
			500	306	93	97	4			
1	G	61	Total	C	N	O	S	0	0	1
			465	286	88	87	4			
1	H	63	Total	C	N	O	S	0	0	1
			477	294	90	89	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	92	Total	O	0	0
			92	92		
2	C	89	Total	O	0	0
			89	89		
2	D	81	Total	O	0	0
			81	81		
2	E	67	Total	O	0	0
			67	67		
2	F	67	Total	O	0	0
			67	67		

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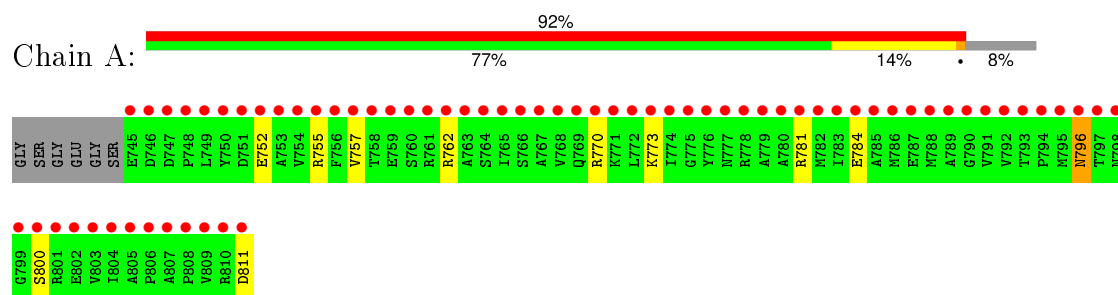
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	97	Total	O	0	0
			97	97		
2	H	74	Total	O	0	0
			74	74		

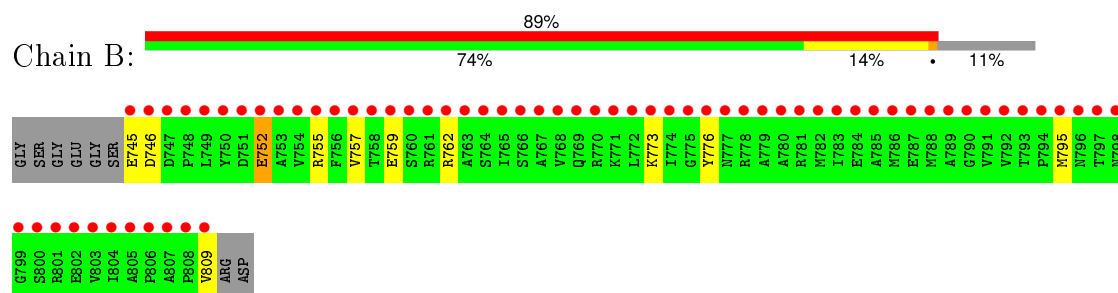
3 Residue-property plots [i](#)

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

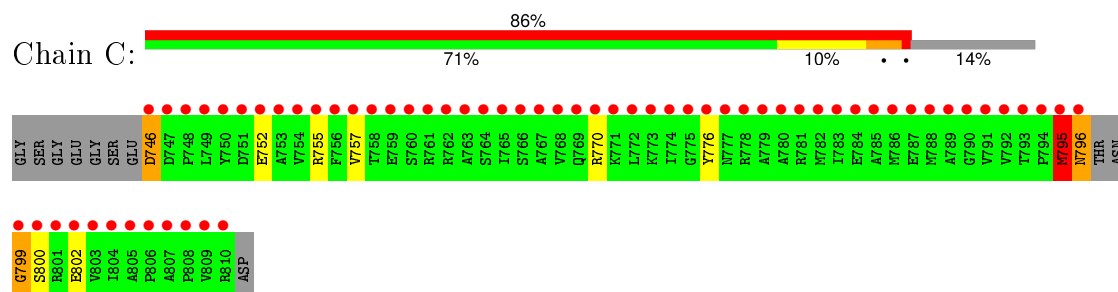
• Molecule 1: DNA TRANSLOCASE FTSK



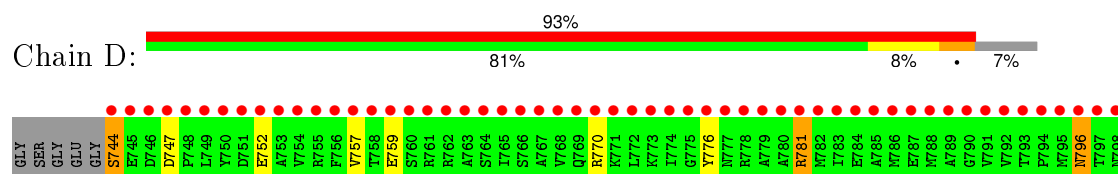
• Molecule 1: DNA TRANSLOCASE FTSK

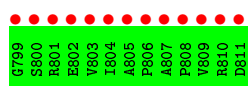


• Molecule 1: DNA TRANSLOCASE FTSK

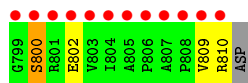
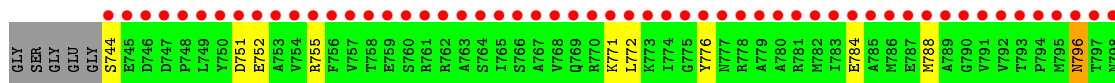
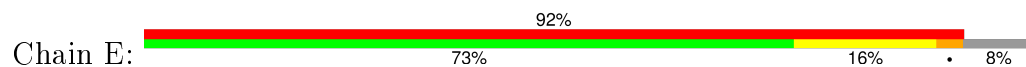


• Molecule 1: DNA TRANSLOCASE FTSK

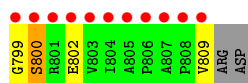
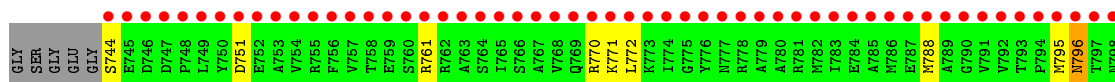
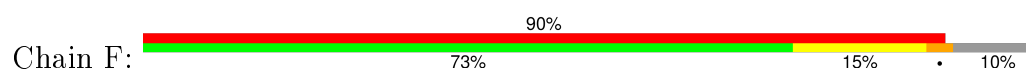




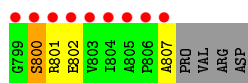
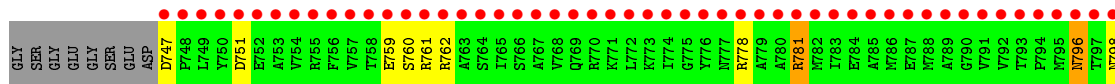
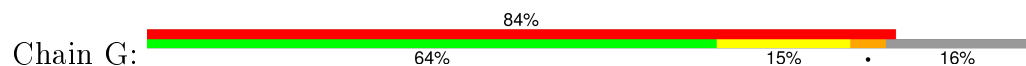
• Molecule 1: DNA TRANSLOCASE FTSK



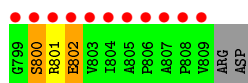
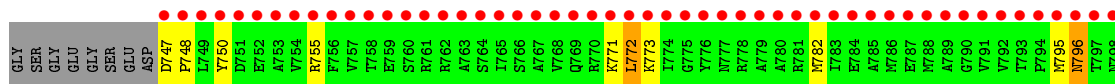
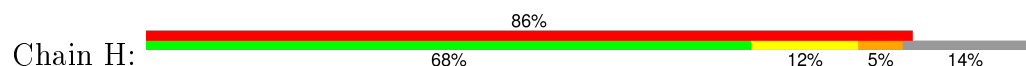
• Molecule 1: DNA TRANSLOCASE FTSK



• Molecule 1: DNA TRANSLOCASE FTSK



• Molecule 1: DNA TRANSLOCASE FTSK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.49Å 58.50Å 95.41Å 90.00° 92.51° 90.00°	Depositor
Resolution (Å)	95.35 – 1.40 40.98 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (95.35-1.40) 43.6 (40.98-1.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.144 , 0.192 0.144 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	2.91 , 99.9	EDS
Estimated twinning fraction	None for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 47818 reflections	Xtriage
F_o, F_c correlation	0.12	EDS
Total number of atoms	4633	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.59% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.41	3/526 (0.6%)	1.28	2/708 (0.3%)
1	B	1.41	3/506 (0.6%)	1.21	0/683
1	C	1.45	5/482 (1.0%)	1.15	1/649 (0.2%)
1	D	1.37	3/532 (0.6%)	1.17	3/716 (0.4%)
1	E	1.54	7/513 (1.4%)	1.28	6/693 (0.9%)
1	F	1.56	5/506 (1.0%)	1.51	5/683 (0.7%)
1	G	1.69	10/470 (2.1%)	1.44	8/633 (1.3%)
1	H	1.38	3/483 (0.6%)	1.29	6/652 (0.9%)
All	All	1.48	39/4018 (1.0%)	1.29	31/5417 (0.6%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	802	GLU	CG-CD	11.83	1.69	1.51
1	G	802	GLU	CD-OE1	9.96	1.36	1.25
1	G	802	GLU	CG-CD	9.81	1.66	1.51
1	A	757	VAL	CB-CG2	-9.71	1.32	1.52
1	E	802	GLU	CG-CD	9.01	1.65	1.51
1	G	802	GLU	CD-OE2	8.25	1.34	1.25
1	G	762	ARG	CZ-NH1	7.69	1.43	1.33
1	C	746	ASP	CB-CG	7.40	1.67	1.51
1	F	802	GLU	CD-OE1	6.96	1.33	1.25
1	D	757	VAL	CB-CG1	-6.84	1.38	1.52
1	F	800	SER	CB-OG	-6.82	1.33	1.42
1	B	776	TYR	CD2-CE2	6.80	1.49	1.39
1	G	762	ARG	CZ-NH2	6.79	1.41	1.33
1	C	795	MET	CB-CG	6.69	1.72	1.51
1	B	752	GLU	CG-CD	6.61	1.61	1.51
1	B	757	VAL	CB-CG1	-6.24	1.39	1.52
1	G	801	ARG	CZ-NH1	6.23	1.41	1.33
1	D	759	GLU	CD-OE1	6.10	1.32	1.25
1	D	776	TYR	CD2-CE2	6.09	1.48	1.39
1	E	752	GLU	CG-CD	6.05	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	802	GLU	CD-OE2	5.97	1.32	1.25
1	E	800	SER	CA-CB	5.88	1.61	1.52
1	H	750	TYR	CE2-CZ	-5.85	1.30	1.38
1	C	776	TYR	CD2-CE2	5.80	1.48	1.39
1	F	751	ASP	CB-CG	5.68	1.63	1.51
1	G	760	SER	CB-OG	5.57	1.49	1.42
1	C	776	TYR	CE2-CZ	-5.49	1.31	1.38
1	G	802	GLU	CB-CG	5.49	1.62	1.52
1	C	799	GLY	N-CA	5.47	1.54	1.46
1	H	800	SER	CB-OG	-5.44	1.35	1.42
1	E	752	GLU	CD-OE1	5.41	1.31	1.25
1	G	759	GLU	CG-CD	5.34	1.59	1.51
1	H	802	GLU	CG-CD	-5.33	1.44	1.51
1	A	755	ARG	CG-CD	5.25	1.65	1.51
1	E	776	TYR	CD2-CE2	5.25	1.47	1.39
1	G	800	SER	CA-CB	5.23	1.60	1.52
1	E	802	GLU	CB-CG	5.22	1.62	1.52
1	F	802	GLU	CD-OE2	5.21	1.31	1.25
1	A	784	GLU	CD-OE1	5.10	1.31	1.25

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	751	ASP	CB-CG-OD2	14.74	131.57	118.30
1	F	770	ARG	NE-CZ-NH2	11.57	126.09	120.30
1	F	751	ASP	CB-CG-OD1	-9.85	109.44	118.30
1	H	801	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	F	770	ARG	NE-CZ-NH1	-8.57	116.02	120.30
1	G	751	ASP	CB-CG-OD2	8.48	125.93	118.30
1	G	762	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	E	751	ASP	CB-CG-OD2	8.45	125.90	118.30
1	G	801	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	E	751	ASP	CB-CG-OD1	-7.85	111.24	118.30
1	H	772	LEU	CB-CG-CD2	-7.39	98.43	111.00
1	C	757	VAL	CG1-CB-CG2	7.03	122.15	110.90
1	D	781	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	H	755	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	G	778	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	E	755	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	G	781	ARG	NE-CZ-NH2	6.39	123.49	120.30
1	E	788	MET	CG-SD-CE	6.25	110.19	100.20
1	A	755	ARG	CG-CD-NE	-6.00	99.21	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	802	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	G	761	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	H	773	LYS	CD-CE-NZ	5.75	124.93	111.70
1	H	782	MET	CG-SD-CE	5.74	109.38	100.20
1	A	781	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	G	762	ARG	NH1-CZ-NH2	5.52	125.47	119.40
1	E	802	GLU	CG-CD-OE2	5.42	129.14	118.30
1	G	801	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	D	747	ASP	CB-CG-OD2	5.38	123.14	118.30
1	H	772	LEU	CB-CG-CD1	5.29	120.00	111.00
1	F	761	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	770	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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	520	0	522	9	0
1	B	500	0	505	9	0
1	C	477	0	485	15	1
1	D	526	0	527	7	0
1	E	507	0	510	8	0
1	F	500	0	501	10	0
1	G	465	0	474	8	0
1	H	477	0	486	12	1
2	A	94	0	0	4	0
2	B	92	0	0	5	0
2	C	89	0	0	9	0
2	D	81	0	0	5	0
2	E	67	0	0	3	0
2	F	67	0	0	3	0
2	G	97	0	0	4	0
2	H	74	0	0	5	0
All	All	4633	0	4010	71	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 9.

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:D:744:SER:HB2	2:D:2001:HOH:O	1.15	1.29
1:B:809:VAL:C	2:B:2092:HOH:O	1.72	1.26
1:H:802:GLU:CD	2:H:2063:HOH:O	1.76	1.21
1:H:802:GLU:OE2	2:H:2062:HOH:O	1.60	1.18
1:H:802:GLU:OE1	2:H:2063:HOH:O	1.63	1.12
1:B:752:GLU:HB2	1:C:752:GLU:OE1	1.54	1.07
1:D:752:GLU:OE1	2:D:2021:HOH:O	1.73	1.07
1:H:802:GLU:OE2	2:H:2063:HOH:O	1.68	1.06
1:F:744:SER:N	2:F:2002:HOH:O	1.85	1.06
1:E:744:SER:N	2:E:2001:HOH:O	1.98	0.95
1:C:796:ASN:HB3	2:C:2064:HOH:O	1.65	0.94
1:C:746:ASP:N	2:C:2006:HOH:O	2.06	0.89
1:G:747:ASP:N	2:G:2005:HOH:O	2.06	0.87
1:C:800:SER:HB2	2:C:2070:HOH:O	1.81	0.79
1:H:747:ASP:N	2:H:2001:HOH:O	2.17	0.77
1:F:809:VAL:N	2:F:2066:HOH:O	2.18	0.76
1:C:796:ASN:HD22	1:C:796:ASN:C	1.88	0.75
1:A:770:ARG:NH2	2:A:2047:HOH:O	2.19	0.75
1:C:795:MET:SD	2:C:2089:HOH:O	2.45	0.74
1:D:781:ARG:HD2	2:D:2047:HOH:O	1.87	0.74
1:A:752:GLU:HB2	1:D:752:GLU:OE2	1.91	0.70
1:D:744:SER:CB	2:D:2001:HOH:O	1.96	0.68
1:A:773:LYS:NZ	2:A:2050:HOH:O	2.09	0.67
1:E:771:LYS:HG3	1:E:772:LEU:HD22	1.80	0.63
1:F:795:MET:HG2	1:F:799:GLY:HA2	1.81	0.62
1:F:795:MET:HE1	1:H:795:MET:HG2	1.82	0.61
1:B:773:LYS:NZ	2:B:2046:HOH:O	2.22	0.60
1:A:796:ASN:ND2	1:A:800:SER:H	1.98	0.60
1:H:796:ASN:C	1:H:796:ASN:HD22	2.05	0.60
1:B:762:ARG:HD3	2:B:2033:HOH:O	2.03	0.58
1:F:788:MET:SD	2:F:2016:HOH:O	2.57	0.58
1:E:796:ASN:C	1:E:796:ASN:HD22	2.05	0.57
1:C:795:MET:HE3	1:C:800:SER:HA	1.89	0.54
1:G:796:ASN:HD22	1:G:796:ASN:C	2.10	0.54
1:C:800:SER:CB	2:C:2070:HOH:O	2.49	0.54
1:A:811:ASP:C	1:A:811:ASP:OD1	2.47	0.53
1:C:795:MET:HE2	1:C:799:GLY:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:771:LYS:CG	1:E:772:LEU:HD22	2.40	0.52
1:F:771:LYS:HG3	1:F:772:LEU:HD22	1.91	0.52
1:D:796:ASN:C	1:D:796:ASN:HD22	2.14	0.51
1:F:796:ASN:HD22	1:F:796:ASN:C	2.12	0.51
1:G:781:ARG:NH1	2:G:2059:HOH:O	2.44	0.50
1:A:762:ARG:NE	2:A:2038:HOH:O	2.44	0.49
1:E:809:VAL:HG23	1:E:810:ARG:N	2.28	0.49
1:F:795:MET:HE3	1:H:795:MET:CE	2.43	0.49
1:D:781:ARG:NH2	2:D:2047:HOH:O	2.10	0.48
1:C:795:MET:CB	2:C:2089:HOH:O	2.61	0.48
1:A:796:ASN:HD22	1:A:796:ASN:C	2.17	0.48
1:A:811:ASP:OXT	1:C:755:ARG:NH1	2.38	0.48
1:C:795:MET:HB2	2:C:2089:HOH:O	2.14	0.47
1:B:745:GLU:CA	2:B:2005:HOH:O	2.62	0.47
1:C:795:MET:CG	2:C:2089:HOH:O	2.64	0.46
1:C:770:ARG:NH2	2:C:2038:HOH:O	2.07	0.46
1:H:796:ASN:ND2	1:H:800:SER:H	2.15	0.45
1:G:796:ASN:ND2	1:G:800:SER:H	2.14	0.45
1:E:784:GLU:HG3	2:E:2046:HOH:O	2.17	0.45
1:F:795:MET:HE3	1:H:795:MET:SD	2.57	0.45
1:H:771:LYS:HG3	1:H:772:LEU:HD12	1.99	0.45
1:G:747:ASP:N	2:G:2008:HOH:O	2.49	0.45
1:G:807:ALA:N	2:G:2090:HOH:O	2.49	0.44
1:B:746:ASP:OD2	1:H:771:LYS:NZ	2.49	0.43
1:B:795:MET:HE3	1:B:795:MET:HB3	1.71	0.43
1:C:795:MET:HE3	1:C:800:SER:CA	2.49	0.43
1:F:796:ASN:ND2	1:F:800:SER:H	2.17	0.42
1:B:745:GLU:N	2:B:2005:HOH:O	2.53	0.41
1:E:796:ASN:ND2	1:E:800:SER:H	2.18	0.41
1:E:744:SER:CA	2:E:2001:HOH:O	2.58	0.41
1:B:755:ARG:O	1:B:759:GLU:HG3	2.21	0.41
1:A:762:ARG:HB2	2:A:2038:HOH:O	2.21	0.41
1:G:796:ASN:C	1:G:796:ASN:ND2	2.74	0.40
1:G:796:ASN:ND2	1:G:798:ASN:H	2.19	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:C:802:GLU:OE1	1:H:748:PRO:CB[1_655]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	65/73 (89%)	65 (100%)	0	0	100	100
1	B	63/73 (86%)	63 (100%)	0	0	100	100
1	C	59/73 (81%)	59 (100%)	0	0	100	100
1	D	66/73 (90%)	66 (100%)	0	0	100	100
1	E	65/73 (89%)	65 (100%)	0	0	100	100
1	F	64/73 (88%)	63 (98%)	1 (2%)	0	100	100
1	G	59/73 (81%)	59 (100%)	0	0	100	100
1	H	61/73 (84%)	60 (98%)	1 (2%)	0	100	100
All	All	502/584 (86%)	500 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	55/58 (95%)	54 (98%)	1 (2%)	66	32
1	B	53/58 (91%)	53 (100%)	0	100	100
1	C	50/58 (86%)	48 (96%)	2 (4%)	38	6
1	D	56/58 (97%)	54 (96%)	2 (4%)	42	9
1	E	54/58 (93%)	53 (98%)	1 (2%)	65	29
1	F	53/58 (91%)	52 (98%)	1 (2%)	65	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	49/58 (84%)	48 (98%)	1 (2%)	63	27
1	H	50/58 (86%)	49 (98%)	1 (2%)	63	27
All	All	420/464 (90%)	411 (98%)	9 (2%)	61	24

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	796	ASN
1	C	795	MET
1	C	796	ASN
1	D	744	SER
1	D	796	ASN
1	E	796	ASN
1	F	796	ASN
1	G	796	ASN
1	H	796	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	777	ASN
1	A	796	ASN
1	C	777	ASN
1	C	796	ASN
1	D	777	ASN
1	D	796	ASN
1	E	777	ASN
1	E	796	ASN
1	F	777	ASN
1	F	796	ASN
1	G	777	ASN
1	G	796	ASN
1	H	777	ASN
1	H	796	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	67/73 (91%)	63.09	67 (100%) 0 0	9, 12, 27, 34	0
1	B	65/73 (89%)	63.73	65 (100%) 0 0	10, 13, 23, 35	0
1	C	63/73 (86%)	66.21	63 (100%) 0 0	8, 14, 28, 35	0
1	D	68/73 (93%)	69.15	68 (100%) 0 0	11, 17, 27, 37	0
1	E	67/73 (91%)	61.57	67 (100%) 0 0	8, 14, 23, 35	0
1	F	66/73 (90%)	66.02	66 (100%) 0 0	10, 16, 26, 39	0
1	G	61/73 (83%)	68.92	61 (100%) 0 0	10, 15, 23, 26	0
1	H	63/73 (86%)	72.03	63 (100%) 0 0	11, 17, 25, 27	0
All	All	520/584 (89%)	66.28	520 (100%) 0 0	8, 15, 27, 39	0

All (520) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	807	ALA	124.3
1	H	750	TYR	117.2
1	D	765	ILE	109.5
1	D	804	ILE	109.4
1	G	750	TYR	108.0
1	H	749	LEU	107.5
1	G	806	PRO	105.9
1	F	776	TYR	105.0
1	H	765	ILE	104.2
1	E	807	ALA	104.2
1	H	804	ILE	103.6
1	H	783	ILE	103.1
1	C	804	ILE	103.0
1	H	754	VAL	102.9
1	H	776	TYR	102.3
1	H	774	ILE	102.0

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Mol	Chain	Res	Type	RSRZ
1	F	749	LEU	100.7
1	D	756	PHE	100.2
1	H	805	ALA	99.9
1	C	756	PHE	99.8
1	F	774	ILE	99.8
1	F	750	TYR	98.4
1	H	791	VAL	98.2
1	E	765	ILE	98.2
1	F	765	ILE	98.0
1	B	804	ILE	97.6
1	D	803	VAL	97.3
1	D	792	VAL	97.0
1	G	756	PHE	96.6
1	G	774	ILE	96.1
1	A	756	PHE	95.9
1	G	772	LEU	95.5
1	G	765	ILE	95.2
1	A	804	ILE	95.2
1	C	792	VAL	95.1
1	H	756	PHE	95.1
1	C	803	VAL	94.7
1	G	803	VAL	94.4
1	E	804	ILE	94.2
1	G	804	ILE	94.2
1	E	776	TYR	94.0
1	D	809	VAL	93.9
1	C	765	ILE	93.6
1	B	765	ILE	93.5
1	D	772	LEU	93.3
1	H	792	VAL	93.3
1	F	807	ALA	93.1
1	F	768	VAL	93.1
1	C	791	VAL	93.0
1	A	809	VAL	92.7
1	G	783	ILE	92.6
1	D	783	ILE	92.4
1	G	776	TYR	92.3
1	H	757	VAL	92.2
1	F	756	PHE	91.7
1	H	772	LEU	91.6
1	A	765	ILE	91.3
1	A	799	GLY	91.2

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Mol	Chain	Res	Type	RSRZ
1	G	805	ALA	91.2
1	F	783	ILE	91.0
1	B	803	VAL	91.0
1	B	776	TYR	91.0
1	E	783	ILE	90.9
1	H	768	VAL	90.9
1	D	763	ALA	90.6
1	D	776	TYR	90.5
1	G	754	VAL	90.4
1	E	774	ILE	90.2
1	C	807	ALA	90.2
1	G	749	LEU	90.1
1	G	791	VAL	90.1
1	D	750	TYR	90.0
1	D	791	VAL	89.9
1	H	797	THR	89.8
1	B	756	PHE	89.2
1	D	768	VAL	88.6
1	D	774	ILE	88.5
1	E	756	PHE	88.1
1	F	805	ALA	87.9
1	G	792	VAL	87.8
1	B	774	ILE	87.4
1	F	772	LEU	87.3
1	D	793	THR	87.1
1	D	807	ALA	86.9
1	C	783	ILE	86.9
1	C	794	PRO	86.8
1	D	757	VAL	86.6
1	F	797	THR	86.4
1	C	763	ALA	86.1
1	B	783	ILE	86.0
1	E	772	LEU	86.0
1	C	754	VAL	85.8
1	B	750	TYR	85.8
1	G	757	VAL	85.7
1	E	749	LEU	85.7
1	H	785	ALA	85.7
1	H	779	ALA	85.6
1	F	791	VAL	85.6
1	A	772	LEU	85.5
1	C	809	VAL	85.3

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Mol	Chain	Res	Type	RSRZ
1	D	749	LEU	85.3
1	C	750	TYR	85.3
1	D	754	VAL	84.9
1	G	768	VAL	84.7
1	C	749	LEU	84.7
1	C	799	GLY	84.4
1	A	791	VAL	84.3
1	H	763	ALA	84.3
1	C	772	LEU	84.1
1	H	807	ALA	84.1
1	B	791	VAL	83.9
1	E	805	ALA	83.7
1	E	808	PRO	83.5
1	A	783	ILE	83.4
1	D	794	PRO	83.3
1	B	792	VAL	83.3
1	B	772	LEU	82.9
1	A	776	TYR	82.7
1	F	792	VAL	82.4
1	C	805	ALA	82.4
1	A	750	TYR	82.1
1	E	768	VAL	82.1
1	F	803	VAL	82.0
1	B	749	LEU	81.9
1	D	808	PRO	81.8
1	H	803	VAL	81.8
1	F	754	VAL	81.7
1	D	800	SER	81.6
1	E	806	PRO	81.2
1	C	774	ILE	80.9
1	C	793	THR	80.8
1	C	808	PRO	80.7
1	A	803	VAL	80.6
1	F	806	PRO	80.5
1	D	785	ALA	80.4
1	D	797	THR	80.4
1	A	763	ALA	80.3
1	F	763	ALA	80.2
1	A	808	PRO	80.2
1	E	791	VAL	80.1
1	C	757	VAL	80.0
1	G	748	PRO	79.8

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Mol	Chain	Res	Type	RSRZ
1	F	785	ALA	79.8
1	F	804	ILE	79.7
1	A	807	ALA	79.7
1	F	757	VAL	79.6
1	B	807	ALA	79.2
1	F	767	ALA	79.2
1	A	792	VAL	79.1
1	E	757	VAL	78.8
1	A	754	VAL	78.7
1	B	763	ALA	78.6
1	B	799	GLY	78.4
1	B	768	VAL	78.4
1	E	792	VAL	78.3
1	A	749	LEU	78.1
1	B	754	VAL	78.1
1	A	757	VAL	77.9
1	C	776	TYR	77.6
1	E	754	VAL	77.6
1	A	768	VAL	77.4
1	D	788	MET	77.3
1	C	806	PRO	77.3
1	D	805	ALA	76.8
1	A	774	ILE	76.8
1	C	788	MET	76.5
1	G	797	THR	76.5
1	H	753	ALA	76.4
1	F	748	PRO	76.4
1	C	768	VAL	76.3
1	E	803	VAL	76.1
1	H	767	ALA	75.9
1	A	795	MET	75.7
1	B	809	VAL	75.6
1	F	780	ALA	75.4
1	D	806	PRO	75.3
1	F	775	GLY	75.3
1	G	799	GLY	75.1
1	F	779	ALA	74.8
1	E	750	TYR	74.7
1	C	785	ALA	74.7
1	H	780	ALA	74.5
1	D	780	ALA	74.5
1	B	757	VAL	74.4

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Mol	Chain	Res	Type	RSRZ
1	A	796	ASN	74.1
1	H	758	THR	74.0
1	D	799	GLY	73.8
1	H	799	GLY	73.6
1	H	793	THR	73.3
1	E	799	GLY	73.1
1	E	767	ALA	72.5
1	C	795	MET	72.5
1	C	767	ALA	72.2
1	A	794	PRO	72.2
1	E	797	THR	71.9
1	G	794	PRO	71.6
1	B	808	PRO	71.4
1	G	763	ALA	71.4
1	D	753	ALA	71.2
1	D	764	SER	70.9
1	F	799	GLY	70.7
1	B	780	ALA	70.6
1	G	758	THR	70.4
1	H	782	MET	70.4
1	G	785	ALA	70.3
1	H	794	PRO	70.2
1	B	767	ALA	70.1
1	C	753	ALA	70.0
1	B	805	ALA	69.9
1	D	779	ALA	69.9
1	E	763	ALA	69.8
1	B	793	THR	69.7
1	D	798	ASN	69.6
1	A	797	THR	69.5
1	B	785	ALA	69.3
1	B	800	SER	69.2
1	G	793	THR	69.2
1	C	789	ALA	69.0
1	F	764	SER	68.7
1	D	758	THR	68.6
1	H	764	SER	68.6
1	H	808	PRO	68.4
1	H	795	MET	68.3
1	A	805	ALA	68.0
1	H	748	PRO	67.8
1	G	753	ALA	67.7

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Mol	Chain	Res	Type	RSRZ
1	G	798	ASN	67.5
1	F	798	ASN	67.4
1	G	780	ALA	67.4
1	A	793	THR	67.4
1	G	795	MET	67.4
1	G	779	ALA	67.4
1	G	747	ASP	67.3
1	G	767	ALA	67.2
1	A	767	ALA	67.2
1	A	753	ALA	67.1
1	B	779	ALA	67.1
1	D	790	GLY	66.9
1	H	775	GLY	66.9
1	F	766	SER	66.7
1	D	810	ARG	66.6
1	F	753	ALA	66.6
1	H	766	SER	66.5
1	C	800	SER	66.4
1	H	778	ARG	66.2
1	E	809	VAL	66.2
1	E	748	PRO	66.1
1	A	806	PRO	65.9
1	F	758	THR	65.9
1	E	780	ALA	65.8
1	C	758	THR	65.7
1	D	789	ALA	65.7
1	D	796	ASN	65.5
1	B	797	THR	65.5
1	H	806	PRO	65.5
1	H	800	SER	65.4
1	D	775	GLY	65.2
1	D	767	ALA	64.8
1	A	785	ALA	64.6
1	H	798	ASN	64.5
1	E	779	ALA	64.2
1	C	790	GLY	64.1
1	F	794	PRO	64.1
1	B	806	PRO	64.0
1	E	793	THR	63.5
1	F	793	THR	63.5
1	B	753	ALA	63.3
1	H	786	MET	63.3

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Mol	Chain	Res	Type	RSRZ
1	E	785	ALA	63.2
1	B	794	PRO	62.9
1	C	780	ALA	62.7
1	E	794	PRO	62.7
1	E	758	THR	62.7
1	D	760	SER	62.3
1	B	758	THR	62.3
1	B	746	ASP	62.2
1	D	746	ASP	62.2
1	F	769	GLN	61.8
1	A	800	SER	61.5
1	F	782	MET	61.4
1	D	748	PRO	61.3
1	B	789	ALA	61.2
1	E	764	SER	61.0
1	E	795	MET	61.0
1	G	766	SER	60.9
1	F	800	SER	60.9
1	A	788	MET	60.8
1	E	798	ASN	60.4
1	B	788	MET	60.4
1	A	758	THR	60.0
1	G	764	SER	60.0
1	F	795	MET	60.0
1	C	764	SER	59.6
1	B	748	PRO	59.4
1	H	796	ASN	59.4
1	A	779	ALA	59.4
1	A	746	ASP	59.3
1	C	760	SER	59.3
1	H	747	ASP	59.2
1	E	766	SER	59.1
1	D	762	ARG	59.1
1	G	789	ALA	59.0
1	C	779	ALA	59.0
1	E	753	ALA	58.9
1	A	780	ALA	58.8
1	B	795	MET	58.5
1	B	775	GLY	58.5
1	C	746	ASP	58.4
1	H	755	ARG	58.3
1	F	808	PRO	58.1

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Mol	Chain	Res	Type	RSRZ
1	B	796	ASN	57.8
1	B	760	SER	57.8
1	H	788	MET	57.7
1	B	751	ASP	57.6
1	H	769	GLN	57.5
1	D	795	MET	57.4
1	D	786	MET	57.2
1	F	789	ALA	57.2
1	D	766	SER	57.0
1	E	775	GLY	56.8
1	A	790	GLY	56.7
1	G	790	GLY	56.3
1	H	762	ARG	56.3
1	B	790	GLY	56.2
1	A	760	SER	56.1
1	C	801	ARG	56.1
1	H	760	SER	56.1
1	E	789	ALA	56.0
1	D	751	ASP	56.0
1	G	760	SER	55.8
1	D	801	ARG	55.8
1	G	775	GLY	55.8
1	F	762	ARG	55.7
1	C	786	MET	55.6
1	G	800	SER	55.6
1	E	790	GLY	55.3
1	H	801	ARG	55.3
1	F	747	ASP	55.2
1	G	796	ASN	55.0
1	A	789	ALA	54.9
1	F	751	ASP	54.9
1	C	802	GLU	54.8
1	F	778	ARG	54.7
1	G	782	MET	54.5
1	H	752	GLU	54.3
1	G	788	MET	54.3
1	H	790	GLY	53.9
1	G	773	LYS	53.9
1	A	762	ARG	53.6
1	C	796	ASN	53.6
1	C	766	SER	53.6
1	D	747	ASP	53.4

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Mol	Chain	Res	Type	RSRZ
1	E	782	MET	53.4
1	G	755	ARG	53.3
1	F	744	SER	53.2
1	H	777	ASN	53.2
1	B	801	ARG	53.1
1	B	764	SER	53.1
1	C	751	ASP	53.0
1	E	800	SER	53.0
1	A	748	PRO	52.9
1	A	811	ASP	52.9
1	C	748	PRO	52.8
1	A	801	ARG	52.7
1	F	760	SER	52.6
1	A	775	GLY	52.6
1	F	801	ARG	52.5
1	F	773	LYS	52.4
1	C	769	GLN	52.4
1	E	769	GLN	52.3
1	F	771	LYS	52.3
1	C	759	GLU	52.3
1	F	770	ARG	52.3
1	G	786	MET	52.3
1	H	751	ASP	52.2
1	A	777	ASN	51.9
1	E	744	SER	51.7
1	E	762	ARG	51.7
1	H	770	ARG	51.6
1	D	770	ARG	51.6
1	F	752	GLU	51.4
1	E	751	ASP	51.4
1	B	786	MET	51.4
1	B	782	MET	51.3
1	F	796	ASN	51.2
1	D	782	MET	51.2
1	H	789	ALA	51.0
1	H	761	ARG	50.9
1	B	762	ARG	50.9
1	A	764	SER	50.8
1	B	770	ARG	50.7
1	D	755	ARG	50.6
1	A	766	SER	50.4
1	D	787	GLU	50.3

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Mol	Chain	Res	Type	RSRZ
1	E	760	SER	50.3
1	B	745	GLU	50.2
1	B	755	ARG	50.2
1	B	798	ASN	50.2
1	C	755	ARG	50.2
1	A	786	MET	50.1
1	G	769	GLN	50.0
1	D	811	ASP	49.8
1	B	747	ASP	49.7
1	H	771	LYS	49.7
1	A	798	ASN	49.7
1	G	752	GLU	49.6
1	D	778	ARG	49.6
1	G	759	GLU	49.5
1	F	790	GLY	49.4
1	A	751	ASP	49.4
1	B	787	GLU	49.4
1	F	745	GLU	49.4
1	C	761	ARG	49.3
1	E	773	LYS	49.3
1	C	775	GLY	49.3
1	H	759	GLU	49.1
1	F	786	MET	49.1
1	E	752	GLU	49.1
1	C	777	ASN	49.0
1	G	761	ARG	48.9
1	E	801	ARG	48.8
1	C	782	MET	48.8
1	G	762	ARG	48.7
1	C	770	ARG	48.7
1	D	761	ARG	48.6
1	H	781	ARG	48.5
1	A	810	ARG	48.5
1	A	802	GLU	48.4
1	G	802	GLU	48.4
1	G	771	LYS	48.3
1	F	788	MET	48.3
1	B	802	GLU	48.2
1	G	801	ARG	48.1
1	A	759	GLU	48.0
1	A	782	MET	48.0
1	G	784	GLU	47.9

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Mol	Chain	Res	Type	RSRZ
1	A	769	GLN	47.8
1	A	755	ARG	47.8
1	E	771	LYS	47.7
1	H	802	GLU	47.5
1	E	747	ASP	47.5
1	D	802	GLU	47.5
1	G	770	ARG	47.4
1	E	796	ASN	47.4
1	B	766	SER	47.3
1	A	787	GLU	47.2
1	A	752	GLU	47.2
1	H	787	GLU	47.2
1	D	745	GLU	47.1
1	D	769	GLN	47.1
1	A	771	LYS	47.0
1	F	759	GLU	46.9
1	D	759	GLU	46.8
1	F	781	ARG	46.8
1	C	787	GLU	46.8
1	E	786	MET	46.7
1	A	781	ARG	46.4
1	G	778	ARG	46.4
1	D	781	ARG	46.3
1	B	778	ARG	46.1
1	H	773	LYS	46.0
1	B	784	GLU	45.8
1	A	747	ASP	45.6
1	D	771	LYS	45.6
1	B	759	GLU	45.5
1	E	761	ARG	45.4
1	B	769	GLN	45.2
1	E	802	GLU	45.2
1	F	755	ARG	45.0
1	C	773	LYS	45.0
1	F	802	GLU	45.0
1	A	773	LYS	45.0
1	E	770	ARG	44.9
1	E	784	GLU	44.8
1	G	781	ARG	44.8
1	B	771	LYS	44.7
1	H	784	GLU	44.7
1	A	770	ARG	44.7

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Mol	Chain	Res	Type	RSRZ
1	G	787	GLU	44.3
1	E	778	ARG	43.6
1	A	778	ARG	43.6
1	C	771	LYS	43.5
1	C	781	ARG	43.5
1	H	809	VAL	43.2
1	D	773	LYS	43.2
1	E	755	ARG	42.7
1	B	761	ARG	42.7
1	F	761	ARG	42.7
1	C	747	ASP	42.6
1	G	751	ASP	42.5
1	A	761	ARG	42.4
1	D	752	GLU	41.4
1	B	773	LYS	41.4
1	G	777	ASN	41.0
1	F	777	ASN	40.8
1	C	778	ARG	40.7
1	E	745	GLU	40.2
1	E	759	GLU	40.1
1	B	752	GLU	40.0
1	D	784	GLU	39.6
1	C	752	GLU	39.5
1	A	745	GLU	38.8
1	E	788	MET	38.7
1	B	781	ARG	38.3
1	E	781	ARG	37.9
1	C	762	ARG	37.9
1	D	744	SER	37.3
1	B	777	ASN	36.3
1	E	777	ASN	36.2
1	F	787	GLU	35.4
1	F	784	GLU	34.8
1	D	777	ASN	34.3
1	E	787	GLU	34.0
1	F	746	ASP	34.0
1	C	784	GLU	32.1
1	A	784	GLU	31.4
1	E	746	ASP	27.3
1	C	810	ARG	14.9
1	F	809	VAL	13.0
1	E	810	ARG	5.7

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.