Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:08 PM GMT

PDB ID	:	4NPQ
Title	:	The resting-state conformation of the GLIC ligand-gated ion channel
Authors	:	Sauguet, L.; Shahsavar, A; Poitevin, F.; Huon, C.; Menny, A.; Nemecz, A.; Haouz, A.; Changeux, J.P.; Corringer, P.J.; Delarue, M.
Deposited on	:	2013-11-22
Resolution	:	4.35 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

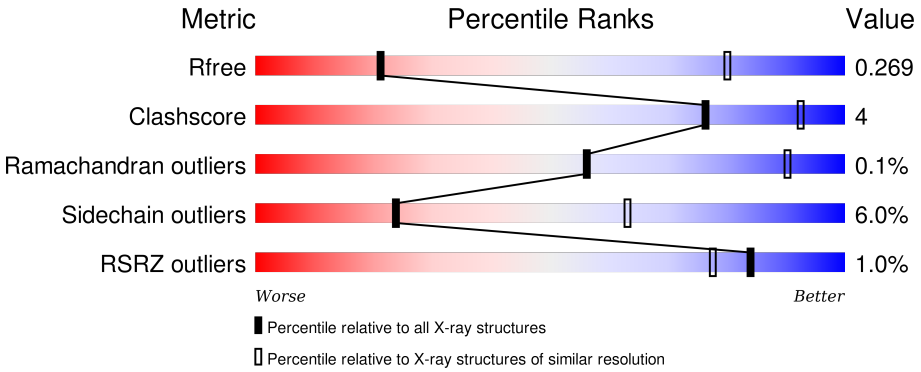
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.35 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}	91344	1063 (5.08-3.60)
Clashscore	102246	1171 (5.08-3.60)
Ramachandran outliers	100387	1110 (5.08-3.60)
Sidechain outliers	100360	1093 (5.08-3.60)
RSRZ outliers	91569	1067 (5.08-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	318	85% 12%
1	B	318	84% 14%
1	C	318	% 84% 13%
1	D	318	% 83% 14%
1	E	318	84% 13%

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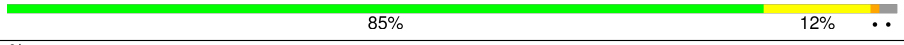
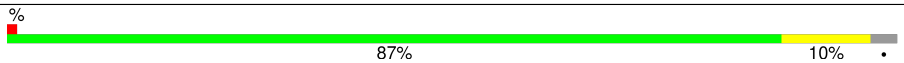
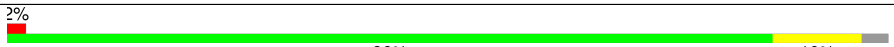
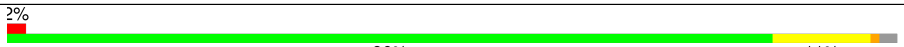
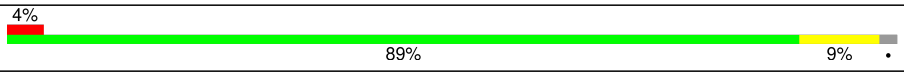
Mol	Chain	Length	Quality of chain
1	F	318	
1	G	318	
1	H	318	
1	I	318	
1	J	318	
1	K	318	
1	L	318	
1	M	318	
1	N	318	
1	O	318	
1	P	318	
1	Q	318	
1	R	318	
1	S	318	
1	T	318	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 45859 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 Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2322	1533	355	430	4			
1	B	311	Total	C	N	O	S	0	0	0
			2334	1540	361	429	4			
1	C	311	Total	C	N	O	S	0	0	0
			2341	1551	359	427	4			
1	D	311	Total	C	N	O	S	0	0	0
			2330	1543	353	431	3			
1	E	311	Total	C	N	O	S	0	0	0
			2355	1559	359	433	4			
1	F	311	Total	C	N	O	S	0	0	0
			2334	1546	361	423	4			
1	G	311	Total	C	N	O	S	0	0	0
			2325	1538	361	422	4			
1	H	309	Total	C	N	O	S	0	0	0
			2199	1440	350	406	3			
1	I	307	Total	C	N	O	S	0	0	0
			2145	1408	344	389	4			
1	J	311	Total	C	N	O	S	0	0	0
			2257	1485	362	407	3			
1	K	309	Total	C	N	O	S	0	0	0
			2312	1530	360	418	4			
1	L	302	Total	C	N	O	S	0	0	0
			2274	1505	344	421	4			
1	M	308	Total	C	N	O	S	0	0	0
			2271	1501	353	413	4			
1	N	311	Total	C	N	O	S	0	0	0
			2359	1564	364	427	4			
1	O	311	Total	C	N	O	S	0	0	0
			2366	1565	362	435	4			
1	P	311	Total	C	N	O	S	0	0	0
			2280	1499	357	420	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	311	Total	C	N	O	S	0	0	0
			2345	1555	357	429	4			
1	R	311	Total	C	N	O	S	0	0	0
			2293	1511	362	417	3			
1	S	309	Total	C	N	O	S	0	0	0
			2268	1497	359	408	4			
1	T	311	Total	C	N	O	S	0	0	0
			2149	1410	352	384	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
A	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
B	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
B	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
C	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
C	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
D	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
D	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
E	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
E	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
F	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
F	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
G	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
G	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
H	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
H	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
I	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
I	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
J	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
J	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
K	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
K	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
L	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
L	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
M	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
M	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
N	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
N	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
O	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
O	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
P	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8

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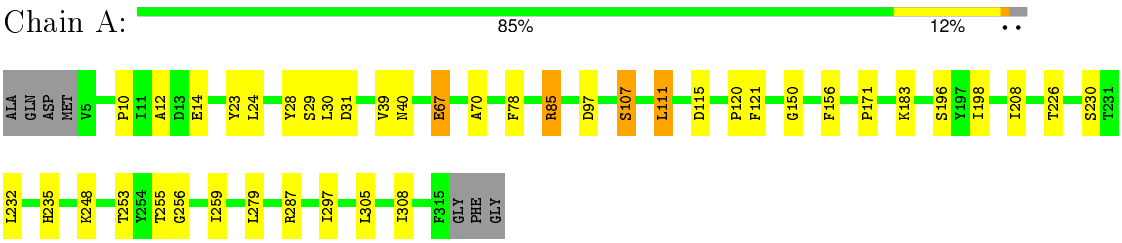
Chain	Residue	Modelled	Actual	Comment	Reference
P	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
Q	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
Q	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
R	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
R	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
S	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
S	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8
T	1	ALA	-	EXPRESSION TAG	UNP Q7NDN8
T	318	GLY	-	EXPRESSION TAG	UNP Q7NDN8

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.

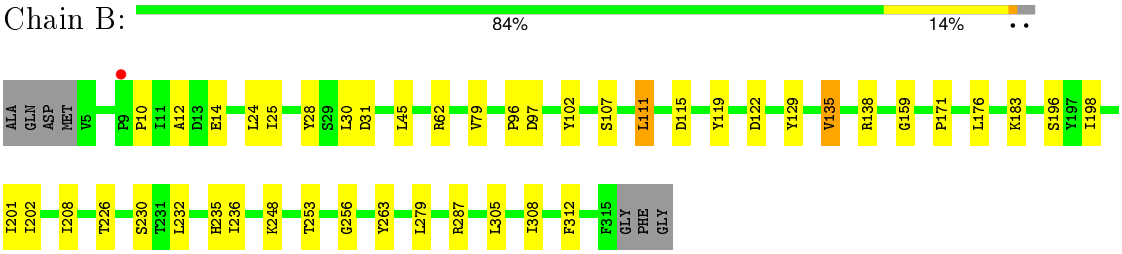
- Molecule 1: Proton-gated ion channel

Chain A:



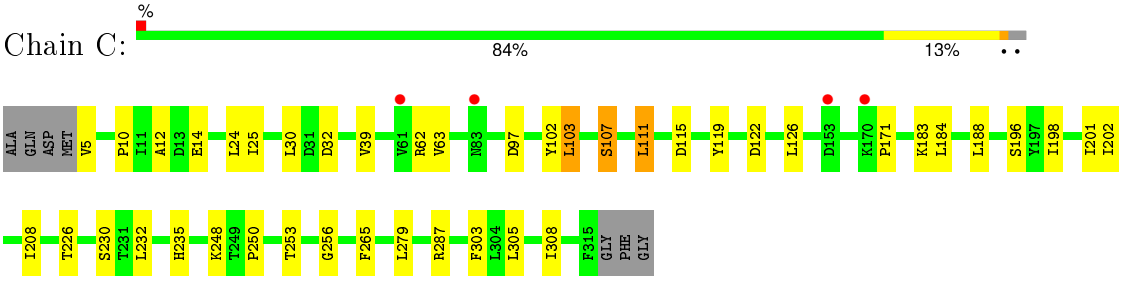
- Molecule 1: Proton-gated ion channel

Chain B:



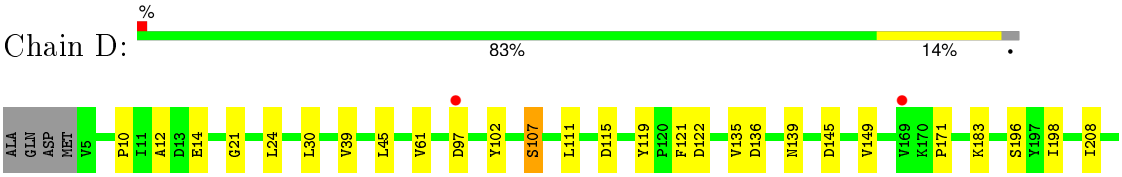
- Molecule 1: Proton-gated ion channel

Chain C:



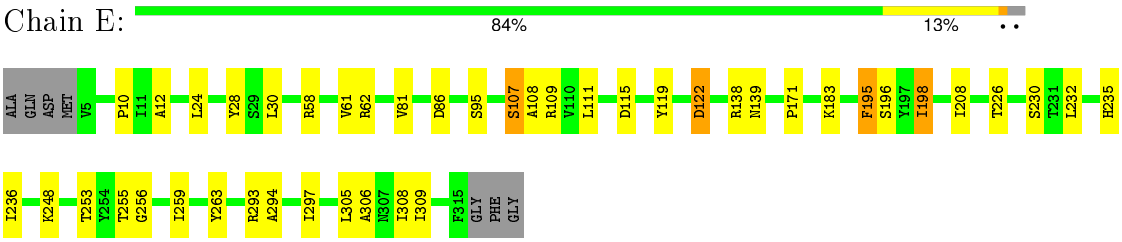
- Molecule 1: Proton-gated ion channel

Chain D:



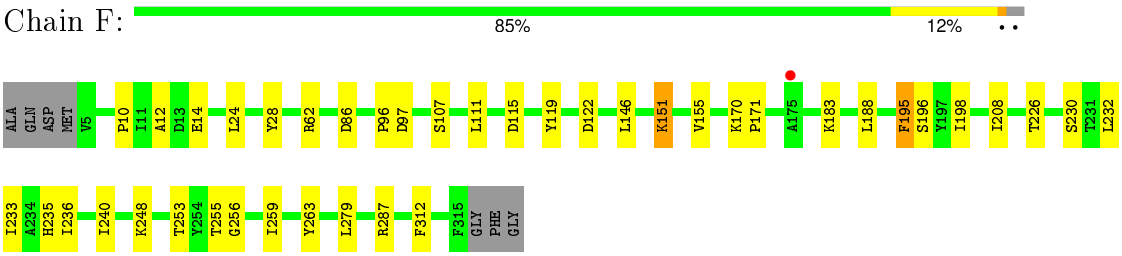
• Molecule 1: Proton-gated ion channel

Chain E:



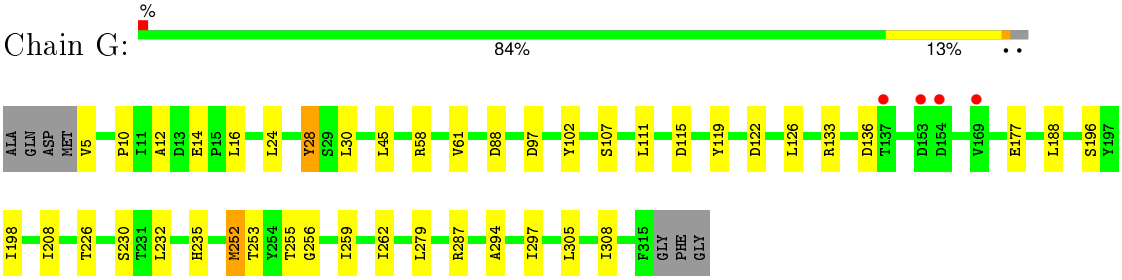
• Molecule 1: Proton-gated ion channel

Chain F:



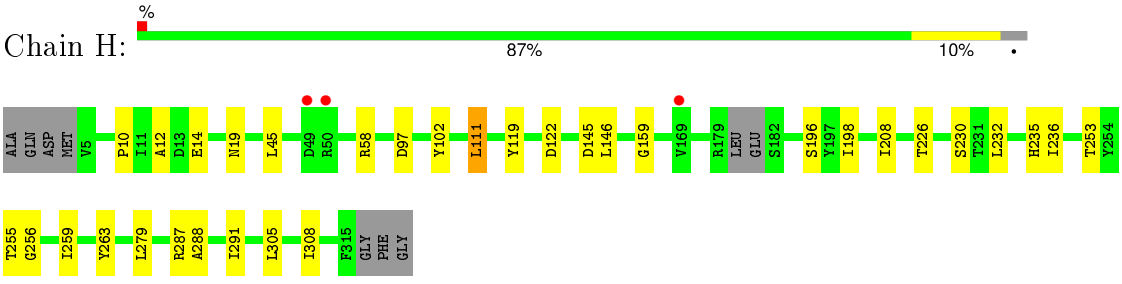
• Molecule 1: Proton-gated ion channel

Chain G:



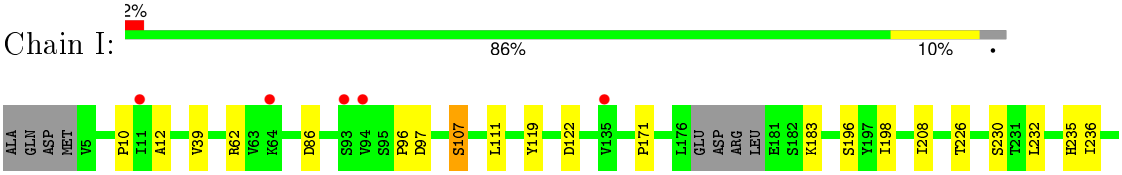
• Molecule 1: Proton-gated ion channel

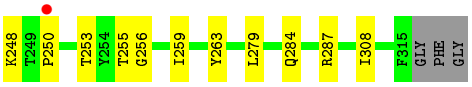
Chain H:



• Molecule 1: Proton-gated ion channel

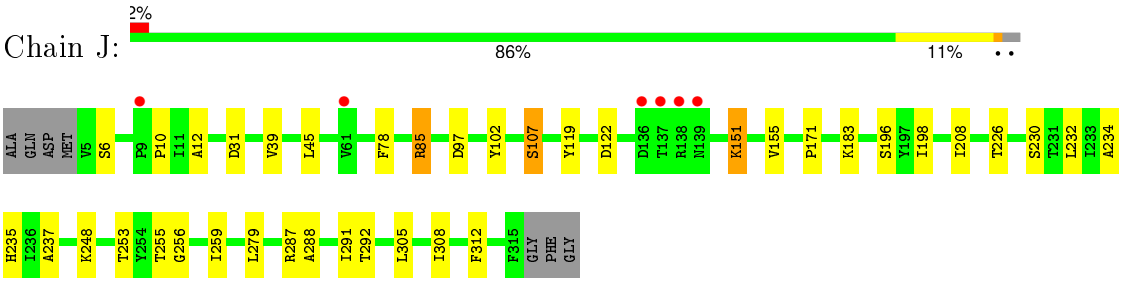
Chain I:





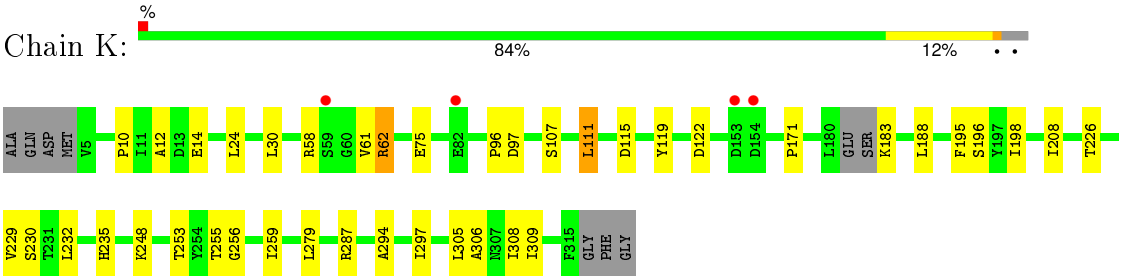
• Molecule 1: Proton-gated ion channel

Chain J:



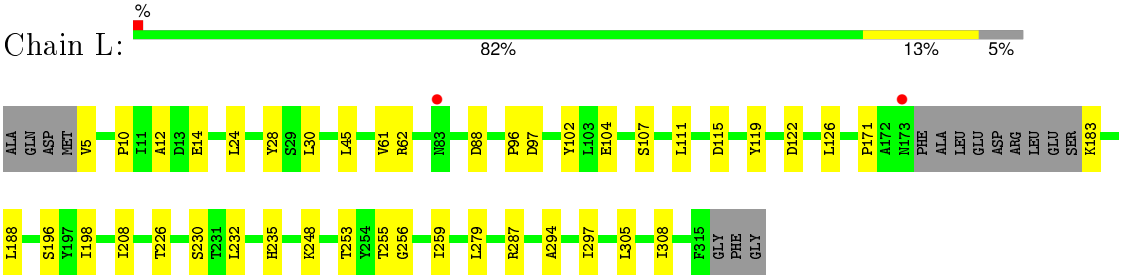
• Molecule 1: Proton-gated ion channel

Chain K:



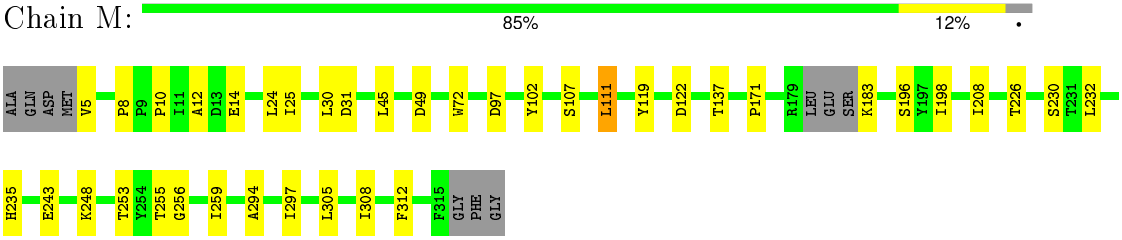
• Molecule 1: Proton-gated ion channel

Chain L:



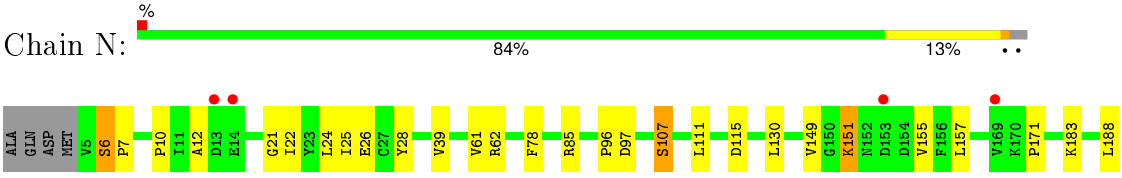
• Molecule 1: Proton-gated ion channel

Chain M:



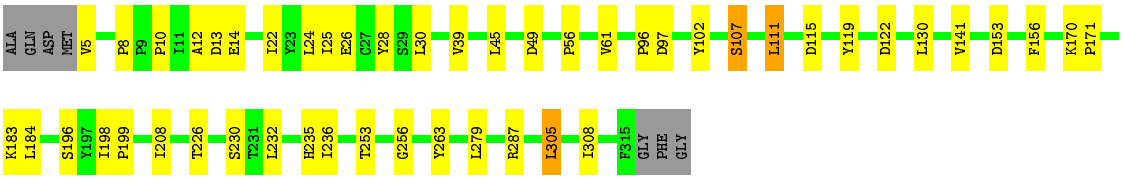
• Molecule 1: Proton-gated ion channel

Chain N:



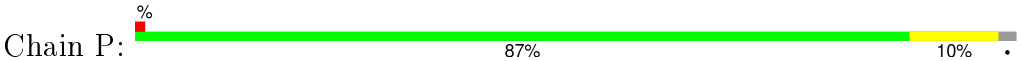
• Molecule 1: Proton-gated ion channel

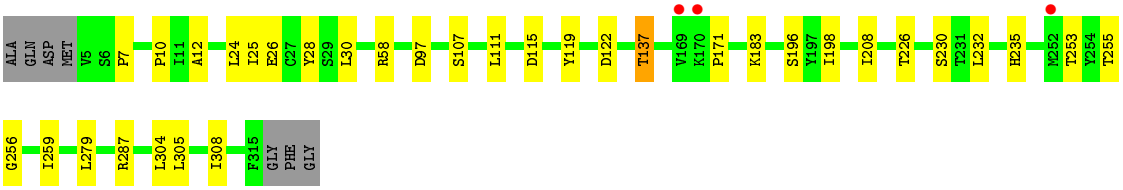
Chain O:



• Molecule 1: Proton-gated ion channel

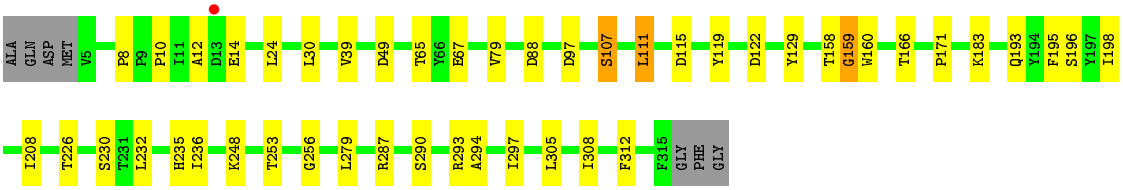
Chain P:





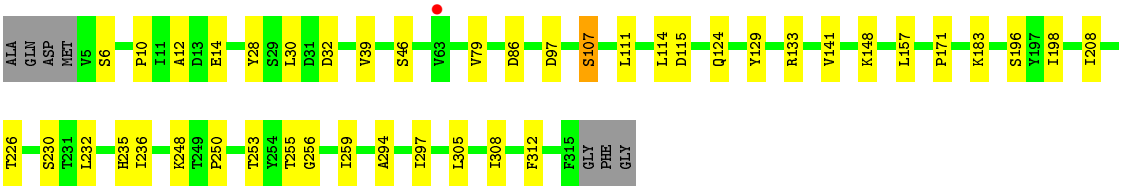
• Molecule 1: Proton-gated ion channel

Chain Q:



• Molecule 1: Proton-gated ion channel

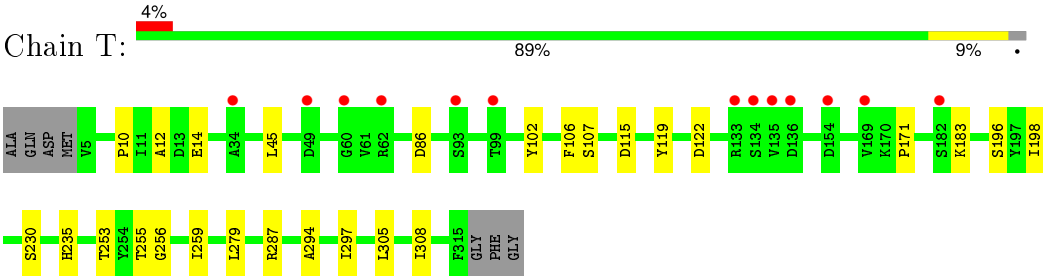
Chain R:



• Molecule 1: Proton-gated ion channel

Chain S:

• Molecule 1: Proton-gated ion channel



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.53Å 384.10Å 148.44Å 90.00° 98.47° 90.00°	Depositor
Resolution (Å)	20.00 – 4.35 20.00 – 4.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-4.35) 99.7 (20.00-4.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 4.36Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.240 , 0.244 0.263 , 0.269	Depositor DCC
R_{free} test set	4700 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	218.1	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 160.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.20$	Xtriage
Outliers	1 of 93884 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	45859	wwPDB-VP
Average B, all atoms (Å^2)	239.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.38	0/2385	0.62	0/3291
1	B	0.40	0/2398	0.63	0/3306
1	C	0.40	0/2406	0.63	0/3317
1	D	0.38	0/2394	0.62	1/3306 (0.0%)
1	E	0.37	0/2419	0.62	0/3335
1	F	0.39	0/2399	0.62	1/3304 (0.0%)
1	G	0.41	0/2389	0.65	0/3293
1	H	0.38	0/2255	0.61	0/3115
1	I	0.38	0/2201	0.62	0/3043
1	J	0.39	0/2318	0.61	0/3197
1	K	0.38	0/2375	0.61	0/3273
1	L	0.36	0/2337	0.59	0/3226
1	M	0.37	0/2333	0.59	0/3221
1	N	0.38	0/2425	0.63	0/3342
1	O	0.37	0/2432	0.62	0/3354
1	P	0.38	0/2342	0.63	0/3234
1	Q	0.39	0/2411	0.63	1/3326 (0.0%)
1	R	0.36	0/2355	0.61	0/3250
1	S	0.37	0/2330	0.59	0/3214
1	T	0.37	0/2206	0.60	0/3050
All	All	0.38	0/47110	0.62	3/64997 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	159	GLY	N-CA-C	-5.49	99.39	113.10
1	F	195	PHE	CA-CB-CG	5.27	126.54	113.90
1	D	121	PHE	N-CA-C	-5.19	96.98	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2322	0	2154	21	0
1	B	2334	0	2173	23	0
1	C	2341	0	2196	20	0
1	D	2330	0	2181	21	0
1	E	2355	0	2213	18	0
1	F	2334	0	2181	22	0
1	G	2325	0	2175	16	0
1	H	2199	0	1930	18	0
1	I	2145	0	1855	15	0
1	J	2257	0	2033	20	0
1	K	2312	0	2156	17	0
1	L	2274	0	2128	21	0
1	M	2271	0	2086	15	0
1	N	2359	0	2238	19	0
1	O	2366	0	2233	29	0
1	P	2280	0	2054	15	0
1	Q	2345	0	2193	26	0
1	R	2293	0	2109	25	0
1	S	2268	0	2072	15	0
1	T	2149	0	1832	13	0
All	All	45859	0	42192	336	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 4.

All (336) 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:L:12:ALA:HB2	1:R:141:VAL:HG11	1.24	1.13
1:H:19:ASN:HB3	1:H:145:ASP:OD1	1.55	1.06
1:L:12:ALA:HB2	1:R:141:VAL:CG1	1.98	0.94
1:Q:10:PRO:HB2	1:Q:12:ALA:O	1.73	0.89
1:L:12:ALA:CB	1:R:141:VAL:HG11	2.03	0.88
1:P:10:PRO:HB2	1:P:12:ALA:O	1.73	0.88
1:E:10:PRO:HB2	1:E:12:ALA:O	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:10:PRO:HB2	1:L:12:ALA:O	1.77	0.84
1:B:10:PRO:HB2	1:B:12:ALA:O	1.78	0.84
1:D:10:PRO:HB2	1:D:12:ALA:O	1.77	0.84
1:M:10:PRO:HB2	1:M:12:ALA:O	1.78	0.84
1:H:10:PRO:HB2	1:H:12:ALA:O	1.78	0.84
1:F:10:PRO:HB2	1:F:12:ALA:O	1.77	0.83
1:C:10:PRO:HB2	1:C:12:ALA:O	1.79	0.83
1:N:10:PRO:HB2	1:N:12:ALA:O	1.77	0.83
1:K:10:PRO:HB2	1:K:12:ALA:O	1.79	0.83
1:J:10:PRO:HB2	1:J:12:ALA:O	1.77	0.83
1:R:10:PRO:HB2	1:R:12:ALA:O	1.78	0.83
1:A:10:PRO:HB2	1:A:12:ALA:O	1.79	0.82
1:L:12:ALA:HB3	1:L:14:GLU:OE1	1.79	0.82
1:I:10:PRO:HB2	1:I:12:ALA:O	1.79	0.82
1:T:10:PRO:HB2	1:T:12:ALA:O	1.80	0.79
1:S:10:PRO:HB2	1:S:12:ALA:O	1.81	0.78
1:G:10:PRO:HB2	1:G:12:ALA:O	1.83	0.78
1:O:22:ILE:HD11	1:O:130:LEU:HD11	1.66	0.77
1:T:12:ALA:HB3	1:T:14:GLU:OE1	1.86	0.76
1:A:12:ALA:HB3	1:A:14:GLU:OE1	1.87	0.75
1:F:151:LYS:HB2	1:F:155:VAL:HG21	1.67	0.75
1:R:12:ALA:HB3	1:R:14:GLU:OE1	1.87	0.75
1:A:111:LEU:HD21	1:E:28:TYR:HB3	1.67	0.74
1:J:151:LYS:HB2	1:J:155:VAL:HG21	1.68	0.74
1:F:12:ALA:HB3	1:F:14:GLU:OE1	1.88	0.74
1:M:12:ALA:HB3	1:M:14:GLU:OE1	1.87	0.74
1:D:12:ALA:HB3	1:D:14:GLU:OE1	1.87	0.74
1:B:305:LEU:O	1:B:308:ILE:HG13	1.88	0.74
1:H:12:ALA:HB3	1:H:14:GLU:OE1	1.87	0.73
1:C:12:ALA:HB3	1:C:14:GLU:OE1	1.88	0.73
1:K:12:ALA:HB3	1:K:14:GLU:OE1	1.87	0.72
1:N:305:LEU:O	1:N:308:ILE:HG13	1.89	0.72
1:G:12:ALA:HB3	1:G:14:GLU:OE1	1.90	0.72
1:N:22:ILE:HD11	1:N:130:LEU:HD11	1.69	0.71
1:B:12:ALA:HB3	1:B:14:GLU:OE1	1.90	0.71
1:E:138:ARG:CA	1:E:139:ASN:N	2.54	0.71
1:Q:158:THR:OG1	1:R:250:PRO:HG3	1.91	0.70
1:F:170:LYS:CB	1:O:170:LYS:CB	2.70	0.70
1:Q:158:THR:C	1:Q:160:TRP:H	1.94	0.69
1:N:151:LYS:HB2	1:N:155:VAL:HG21	1.76	0.68
1:N:6:SER:HB2	1:N:7:PRO:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:305:LEU:O	1:O:308:ILE:HG13	1.94	0.67
1:C:63:VAL:HG23	1:D:136:ASP:HB3	1.75	0.67
1:Q:290:SER:O	1:Q:293:ARG:HG2	1.96	0.66
1:O:8:PRO:HB3	1:O:49:ASP:OD1	1.96	0.65
1:K:111:LEU:HD21	1:O:28:TYR:HB3	1.79	0.65
1:Q:159:GLY:HA2	1:Q:193:GLN:HB2	1.79	0.65
1:O:12:ALA:HB3	1:O:14:GLU:OE1	1.98	0.64
1:M:8:PRO:HB3	1:M:49:ASP:OD1	1.96	0.64
1:Q:8:PRO:HB3	1:Q:49:ASP:OD1	1.98	0.63
1:S:78:PHE:CE2	1:S:85:ARG:HD3	2.34	0.62
1:Q:158:THR:OG1	1:R:250:PRO:CG	2.47	0.62
1:F:146:LEU:CD1	1:O:141:VAL:HG11	2.30	0.62
1:J:288:ALA:O	1:J:291:ILE:HG13	2.00	0.61
1:R:28:TYR:CB	1:S:111:LEU:HD21	2.31	0.61
1:Q:158:THR:C	1:Q:160:TRP:N	2.54	0.60
1:D:288:ALA:O	1:D:291:ILE:HG13	2.02	0.59
1:R:46:SER:HB2	1:R:148:LYS:NZ	2.18	0.59
1:G:28:TYR:HB3	1:H:111:LEU:HD21	1.85	0.59
1:J:78:PHE:CE2	1:J:85:ARG:HD3	2.39	0.58
1:N:6:SER:CB	1:N:7:PRO:CD	2.81	0.58
1:A:23:TYR:HA	1:A:150:GLY:O	2.04	0.58
1:J:78:PHE:HE2	1:J:85:ARG:HD3	1.68	0.57
1:G:235:HIS:CE1	1:G:262:ILE:HG21	2.39	0.57
1:S:78:PHE:HE2	1:S:85:ARG:HD3	1.69	0.56
1:P:28:TYR:CG	1:Q:111:LEU:HD11	2.39	0.56
1:L:28:TYR:HB3	1:M:111:LEU:HD21	1.86	0.56
1:C:208:ILE:HD13	1:C:235:HIS:HB2	1.87	0.56
1:Q:119:TYR:HA	1:Q:122:ASP:OD1	2.06	0.56
1:F:96:PRO:HG2	1:O:96:PRO:HG2	1.87	0.56
1:Q:208:ILE:HD13	1:Q:235:HIS:HB2	1.88	0.55
1:B:135:VAL:HG12	1:B:138:ARG:H	1.70	0.55
1:F:232:LEU:HD21	1:J:208:ILE:HG22	1.87	0.55
1:I:208:ILE:HD13	1:I:235:HIS:HB2	1.88	0.55
1:P:28:TYR:CD1	1:Q:111:LEU:HD11	2.42	0.55
1:E:208:ILE:HD13	1:E:235:HIS:HB2	1.88	0.55
1:A:120:PRO:HD2	1:A:121:PHE:CE2	2.42	0.55
1:T:208:ILE:HD13	1:T:235:HIS:HB2	1.88	0.54
1:L:208:ILE:HD13	1:L:235:HIS:HB2	1.90	0.54
1:F:146:LEU:HD13	1:O:141:VAL:HG11	1.90	0.54
1:M:208:ILE:HD13	1:M:235:HIS:HB2	1.90	0.54
1:P:208:ILE:HD13	1:P:235:HIS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:TYR:HA	1:H:122:ASP:OD1	2.09	0.53
1:R:208:ILE:HD13	1:R:235:HIS:HB2	1.90	0.53
1:D:208:ILE:HD13	1:D:235:HIS:HB2	1.91	0.53
1:D:253:THR:HG23	1:D:256:GLY:H	1.75	0.52
1:O:208:ILE:HD13	1:O:235:HIS:HB2	1.91	0.52
1:O:26:GLU:OE1	1:O:156:PHE:HE1	1.93	0.52
1:N:6:SER:HB2	1:N:7:PRO:CD	2.39	0.52
1:O:253:THR:HG23	1:O:256:GLY:H	1.75	0.52
1:A:208:ILE:HD13	1:A:235:HIS:HB2	1.91	0.52
1:N:208:ILE:HD13	1:N:235:HIS:HB2	1.93	0.51
1:E:119:TYR:HA	1:E:122:ASP:OD1	2.10	0.51
1:F:208:ILE:HD13	1:F:235:HIS:HB2	1.91	0.51
1:H:288:ALA:O	1:H:291:ILE:HG13	2.11	0.51
1:R:253:THR:HG23	1:R:256:GLY:H	1.75	0.51
1:N:253:THR:HG23	1:N:256:GLY:H	1.76	0.51
1:B:253:THR:HG23	1:B:256:GLY:H	1.76	0.51
1:J:253:THR:HG23	1:J:256:GLY:H	1.75	0.51
1:T:253:THR:HG23	1:T:256:GLY:H	1.76	0.51
1:B:28:TYR:HB3	1:C:111:LEU:HD21	1.91	0.51
1:F:253:THR:HG23	1:F:256:GLY:H	1.76	0.51
1:H:19:ASN:HB3	1:H:145:ASP:CG	2.29	0.51
1:G:253:THR:HG23	1:G:256:GLY:H	1.76	0.51
1:H:253:THR:HG23	1:H:256:GLY:H	1.75	0.51
1:H:159:GLY:HA2	1:I:250:PRO:HB2	1.92	0.50
1:B:208:ILE:HG22	1:C:232:LEU:HD21	1.93	0.50
1:Q:253:THR:HG23	1:Q:256:GLY:H	1.76	0.50
1:S:253:THR:HG23	1:S:256:GLY:H	1.76	0.50
1:A:23:TYR:OH	1:B:176:LEU:HA	2.12	0.50
1:L:253:THR:HG23	1:L:256:GLY:H	1.76	0.50
1:J:208:ILE:HD13	1:J:235:HIS:HB2	1.94	0.50
1:S:119:TYR:HA	1:S:122:ASP:OD1	2.12	0.50
1:P:28:TYR:HB3	1:Q:111:LEU:HD21	1.94	0.49
1:C:253:THR:HG23	1:C:256:GLY:H	1.77	0.49
1:P:253:THR:HG23	1:P:256:GLY:H	1.76	0.49
1:F:195:PHE:HE1	1:G:252:MET:HB2	1.77	0.49
1:E:253:THR:HG23	1:E:256:GLY:H	1.76	0.49
1:G:208:ILE:HD13	1:G:235:HIS:HB2	1.93	0.49
1:I:208:ILE:HG22	1:J:232:LEU:HD21	1.95	0.49
1:G:208:ILE:HG22	1:H:232:LEU:HD21	1.94	0.49
1:K:253:THR:HG23	1:K:256:GLY:H	1.77	0.49
1:S:208:ILE:HD13	1:S:235:HIS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG23	1:A:256:GLY:H	1.78	0.49
1:M:253:THR:HG23	1:M:256:GLY:H	1.77	0.49
1:H:208:ILE:HD13	1:H:235:HIS:HB2	1.96	0.48
1:K:208:ILE:HD13	1:K:235:HIS:HB2	1.95	0.48
1:O:198:ILE:HG13	1:O:199:PRO:HD3	1.96	0.48
1:A:156:PHE:HZ	1:B:111:LEU:HD23	1.78	0.48
1:H:159:GLY:CA	1:I:250:PRO:HB2	2.43	0.48
1:K:232:LEU:HD21	1:O:208:ILE:HG22	1.95	0.48
1:P:7:PRO:HG2	1:P:137:THR:OG1	2.13	0.48
1:O:10:PRO:HB2	1:O:13:ASP:H	1.79	0.48
1:I:253:THR:HG23	1:I:256:GLY:H	1.78	0.47
1:D:208:ILE:HG22	1:E:232:LEU:HD21	1.96	0.47
1:D:21:GLY:HA2	1:D:149:VAL:HG22	1.97	0.47
1:B:79:VAL:HG23	1:B:129:TYR:O	2.14	0.47
1:C:119:TYR:HA	1:C:122:ASP:OD1	2.14	0.47
1:F:233:ILE:HD11	1:J:230:SER:O	2.14	0.47
1:B:159:GLY:HA3	1:C:250:PRO:HB2	1.96	0.47
1:N:28:TYR:HB3	1:O:111:LEU:HD21	1.95	0.47
1:O:198:ILE:HG13	1:O:199:PRO:CD	2.45	0.46
1:H:208:ILE:HG22	1:I:232:LEU:HD21	1.97	0.46
1:K:208:ILE:HG22	1:L:232:LEU:HD21	1.97	0.46
1:O:171:PRO:CG	1:O:184:LEU:HA	2.45	0.46
1:C:208:ILE:HG22	1:D:232:LEU:HD21	1.97	0.46
1:P:232:LEU:HD21	1:T:208:ILE:HG22	1.98	0.46
1:A:208:ILE:HG22	1:B:232:LEU:HD21	1.97	0.46
1:F:208:ILE:HG22	1:G:232:LEU:HD21	1.98	0.46
1:F:226:THR:O	1:F:230:SER:HB2	2.16	0.46
1:S:294:ALA:O	1:S:297:ILE:HG13	2.16	0.46
1:A:232:LEU:HD21	1:E:208:ILE:HG22	1.98	0.45
1:F:119:TYR:HA	1:F:122:ASP:OD1	2.17	0.45
1:B:201:ILE:HG22	1:B:202:ILE:HD13	1.98	0.45
1:N:62:ARG:O	1:N:96:PRO:HD3	2.16	0.45
1:Q:171:PRO:HB2	1:Q:183:LYS:O	2.16	0.45
1:C:265:PHE:CE1	1:C:303:PHE:HD2	2.34	0.45
1:A:156:PHE:CZ	1:B:111:LEU:HD23	2.51	0.45
1:M:119:TYR:HA	1:M:122:ASP:OD1	2.16	0.45
1:C:171:PRO:HB2	1:C:183:LYS:O	2.17	0.45
1:E:226:THR:O	1:E:230:SER:HB2	2.17	0.45
1:R:208:ILE:HG22	1:S:232:LEU:HD21	1.99	0.45
1:A:226:THR:O	1:A:230:SER:HB2	2.17	0.45
1:L:208:ILE:HG22	1:M:232:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:226:THR:O	1:S:230:SER:HB2	2.17	0.45
1:D:226:THR:O	1:D:230:SER:HB2	2.17	0.45
1:L:226:THR:O	1:L:230:SER:HB2	2.17	0.45
1:G:226:THR:O	1:G:230:SER:HB2	2.17	0.45
1:F:171:PRO:HB2	1:F:183:LYS:O	2.17	0.45
1:R:226:THR:O	1:R:230:SER:HB2	2.17	0.45
1:B:119:TYR:HA	1:B:122:ASP:OD1	2.17	0.45
1:T:226:THR:O	1:T:230:SER:HB2	2.17	0.45
1:C:226:THR:O	1:C:230:SER:HB2	2.18	0.44
1:P:304:LEU:O	1:P:308:ILE:HG13	2.16	0.44
1:E:86:ASP:HB3	1:E:107:SER:O	2.16	0.44
1:B:226:THR:O	1:B:230:SER:HB2	2.17	0.44
1:K:226:THR:O	1:K:230:SER:HB2	2.18	0.44
1:H:279:LEU:HD13	1:H:287:ARG:HB3	1.99	0.44
1:O:279:LEU:HD13	1:O:287:ARG:HB3	1.99	0.44
1:I:119:TYR:HA	1:I:122:ASP:OD1	2.17	0.44
1:G:119:TYR:HA	1:G:122:ASP:OD1	2.17	0.44
1:R:294:ALA:O	1:R:297:ILE:HG13	2.18	0.44
1:N:226:THR:O	1:N:230:SER:HB2	2.18	0.44
1:J:119:TYR:HA	1:J:122:ASP:OD1	2.17	0.44
1:P:226:THR:O	1:P:230:SER:HB2	2.16	0.44
1:N:171:PRO:HB2	1:N:183:LYS:O	2.18	0.44
1:D:171:PRO:HB2	1:D:183:LYS:O	2.17	0.44
1:O:119:TYR:HA	1:O:122:ASP:OD1	2.18	0.44
1:P:119:TYR:HA	1:P:122:ASP:OD1	2.17	0.44
1:F:62:ARG:HB3	1:O:56:PRO:HD3	1.99	0.44
1:Q:226:THR:O	1:Q:230:SER:HB2	2.17	0.44
1:E:171:PRO:HB2	1:E:183:LYS:O	2.18	0.44
1:E:294:ALA:O	1:E:297:ILE:HG13	2.18	0.44
1:J:226:THR:O	1:J:230:SER:HB2	2.17	0.44
1:T:119:TYR:HA	1:T:122:ASP:OD1	2.18	0.44
1:A:171:PRO:HB2	1:A:183:LYS:O	2.18	0.44
1:A:28:TYR:HE1	1:A:40:ASN:HB2	1.83	0.44
1:K:294:ALA:O	1:K:297:ILE:HG13	2.17	0.43
1:I:226:THR:O	1:I:230:SER:HB2	2.17	0.43
1:L:294:ALA:O	1:L:297:ILE:HG13	2.18	0.43
1:B:279:LEU:HD13	1:B:287:ARG:HB3	1.99	0.43
1:T:294:ALA:O	1:T:297:ILE:HG13	2.19	0.43
1:J:171:PRO:HB2	1:J:183:LYS:O	2.17	0.43
1:B:208:ILE:HD13	1:B:235:HIS:HB2	2.00	0.43
1:O:226:THR:O	1:O:230:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:LEU:HD13	1:G:287:ARG:HB3	1.99	0.43
1:Q:65:THR:HG21	1:R:133:ARG:HH12	1.83	0.43
1:M:226:THR:O	1:M:230:SER:HB2	2.18	0.43
1:A:67:GLU:HG2	1:A:70:ALA:HB2	2.01	0.43
1:L:171:PRO:HB2	1:L:183:LYS:O	2.18	0.43
1:L:12:ALA:CA	1:R:141:VAL:HG11	2.47	0.43
1:Q:158:THR:OG1	1:R:250:PRO:HG2	2.19	0.43
1:O:171:PRO:HB2	1:O:183:LYS:O	2.19	0.43
1:T:279:LEU:HD13	1:T:287:ARG:HB3	2.00	0.43
1:M:208:ILE:HG22	1:N:232:LEU:HD21	2.00	0.43
1:P:171:PRO:HB2	1:P:183:LYS:O	2.19	0.43
1:L:126:LEU:HD12	1:L:188:LEU:HD23	2.00	0.43
1:R:171:PRO:HB2	1:R:183:LYS:O	2.18	0.43
1:R:46:SER:HB2	1:R:148:LYS:HZ1	1.83	0.43
1:D:119:TYR:N	1:D:122:ASP:HB3	2.33	0.43
1:M:294:ALA:O	1:M:297:ILE:HG13	2.19	0.43
1:D:294:ALA:O	1:D:297:ILE:HG13	2.18	0.43
1:K:171:PRO:HB2	1:K:183:LYS:O	2.19	0.43
1:H:226:THR:O	1:H:230:SER:HB2	2.18	0.43
1:E:195:PHE:O	1:E:198:ILE:HD12	2.18	0.43
1:Q:159:GLY:N	1:Q:193:GLN:OE1	2.52	0.43
1:B:171:PRO:HB2	1:B:183:LYS:O	2.19	0.43
1:S:119:TYR:N	1:S:122:ASP:HB3	2.33	0.42
1:K:119:TYR:HA	1:K:122:ASP:OD1	2.19	0.42
1:I:171:PRO:HB2	1:I:183:LYS:O	2.19	0.42
1:Q:279:LEU:HD13	1:Q:287:ARG:HB3	2.01	0.42
1:S:171:PRO:HB2	1:S:183:LYS:O	2.19	0.42
1:P:279:LEU:HD13	1:P:287:ARG:HB3	2.01	0.42
1:N:78:PHE:CE2	1:N:85:ARG:HD3	2.54	0.42
1:Q:294:ALA:O	1:Q:297:ILE:HG13	2.19	0.42
1:F:240:ILE:HD11	1:J:237:ALA:O	2.20	0.42
1:J:279:LEU:HD13	1:J:287:ARG:HB3	2.01	0.42
1:A:78:PHE:CD2	1:A:85:ARG:HG2	2.54	0.42
1:E:81:VAL:HG21	1:E:108:ALA:HB1	2.02	0.42
1:C:201:ILE:HG22	1:C:202:ILE:HD13	1.99	0.42
1:A:78:PHE:CE2	1:A:85:ARG:HG2	2.55	0.42
1:T:86:ASP:O	1:T:106:PHE:HA	2.19	0.42
1:Q:208:ILE:HG22	1:R:232:LEU:HD21	2.02	0.42
1:N:208:ILE:HG22	1:O:232:LEU:HD21	2.01	0.42
1:B:208:ILE:HD11	1:B:235:HIS:HD2	1.85	0.42
1:L:119:TYR:HA	1:L:122:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:159:GLY:CA	1:Q:193:GLN:HB2	2.48	0.42
1:J:291:ILE:HG13	1:J:292:THR:H	1.85	0.42
1:T:171:PRO:HB2	1:T:183:LYS:O	2.19	0.42
1:G:294:ALA:O	1:G:297:ILE:HG13	2.20	0.42
1:C:102:TYR:O	1:C:103:LEU:HD13	2.19	0.42
1:C:126:LEU:HD12	1:C:188:LEU:HD23	2.01	0.42
1:N:279:LEU:HD13	1:N:287:ARG:HB3	2.01	0.42
1:O:22:ILE:HD11	1:O:130:LEU:CD1	2.44	0.41
1:C:171:PRO:CG	1:C:184:LEU:HA	2.50	0.41
1:E:81:VAL:HG23	1:E:109:ARG:O	2.20	0.41
1:H:255:THR:O	1:H:259:ILE:HG12	2.20	0.41
1:A:279:LEU:HD13	1:A:287:ARG:HB3	2.02	0.41
1:L:88:ASP:O	1:L:104:GLU:HB2	2.20	0.41
1:I:255:THR:O	1:I:259:ILE:HG12	2.20	0.41
1:R:255:THR:O	1:R:259:ILE:HG12	2.20	0.41
1:M:171:PRO:HB2	1:M:183:LYS:O	2.19	0.41
1:H:236:ILE:CD1	1:H:263:TYR:HE1	2.33	0.41
1:L:62:ARG:O	1:L:96:PRO:HD3	2.20	0.41
1:Q:39:VAL:O	1:Q:107:SER:HA	2.20	0.41
1:I:236:ILE:CD1	1:I:263:TYR:HE1	2.34	0.41
1:I:62:ARG:O	1:I:96:PRO:HD3	2.19	0.41
1:D:291:ILE:HG13	1:D:292:THR:H	1.85	0.41
1:C:119:TYR:N	1:C:122:ASP:HB3	2.35	0.41
1:F:233:ILE:HG13	1:J:234:ALA:HB2	2.02	0.41
1:P:25:ILE:HG22	1:P:26:GLU:HG2	2.02	0.41
1:F:236:ILE:CD1	1:F:263:TYR:HE1	2.33	0.41
1:F:279:LEU:HD13	1:F:287:ARG:HB3	2.02	0.41
1:L:279:LEU:HD13	1:L:287:ARG:HB3	2.02	0.41
1:S:279:LEU:HD13	1:S:287:ARG:HB3	2.02	0.41
1:H:45:LEU:HB2	1:H:102:TYR:HB3	2.02	0.41
1:A:39:VAL:O	1:A:107:SER:HA	2.20	0.41
1:C:39:VAL:O	1:C:107:SER:HA	2.20	0.41
1:M:255:THR:O	1:M:259:ILE:HG12	2.20	0.41
1:K:119:TYR:N	1:K:122:ASP:HB3	2.35	0.41
1:A:255:THR:O	1:A:259:ILE:HG12	2.21	0.41
1:C:279:LEU:HD13	1:C:287:ARG:HB3	2.02	0.41
1:J:39:VAL:O	1:J:107:SER:HA	2.21	0.41
1:O:236:ILE:CD1	1:O:263:TYR:HE1	2.34	0.41
1:N:21:GLY:HA2	1:N:149:VAL:HG22	2.03	0.41
1:M:45:LEU:HB2	1:M:102:TYR:HB3	2.03	0.41
1:J:255:THR:O	1:J:259:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:THR:O	1:D:259:ILE:HG12	2.20	0.41
1:T:45:LEU:HB2	1:T:102:TYR:HB3	2.03	0.41
1:L:255:THR:O	1:L:259:ILE:HG12	2.21	0.41
1:D:232:LEU:O	1:D:236:ILE:HG12	2.21	0.41
1:K:229:VAL:HG12	1:O:230:SER:HB3	2.02	0.41
1:T:255:THR:O	1:T:259:ILE:HG12	2.21	0.41
1:S:45:LEU:HB2	1:S:102:TYR:HB3	2.03	0.41
1:B:45:LEU:HB2	1:B:102:TYR:HB3	2.03	0.41
1:E:306:ALA:HA	1:E:309:ILE:HD12	2.03	0.41
1:F:255:THR:O	1:F:259:ILE:HG12	2.20	0.41
1:G:126:LEU:HD12	1:G:188:LEU:HD23	2.02	0.41
1:J:45:LEU:HB2	1:J:102:TYR:HB3	2.03	0.41
1:B:62:ARG:O	1:B:96:PRO:HD3	2.21	0.41
1:G:255:THR:O	1:G:259:ILE:HG12	2.21	0.40
1:Q:79:VAL:HB	1:Q:129:TYR:HB2	2.03	0.40
1:E:236:ILE:CD1	1:E:263:TYR:HE1	2.33	0.40
1:I:279:LEU:HD13	1:I:287:ARG:HB3	2.02	0.40
1:S:255:THR:O	1:S:259:ILE:HG12	2.20	0.40
1:D:135:VAL:HG22	1:D:136:ASP:H	1.86	0.40
1:B:236:ILE:CD1	1:B:263:TYR:HE1	2.34	0.40
1:L:45:LEU:HB2	1:L:102:TYR:HB3	2.03	0.40
1:O:39:VAL:O	1:O:107:SER:HA	2.21	0.40
1:O:45:LEU:HB2	1:O:102:TYR:HB3	2.03	0.40
1:K:279:LEU:HD13	1:K:287:ARG:HB3	2.02	0.40
1:D:145:ASP:O	1:D:149:VAL:HG23	2.22	0.40
1:R:39:VAL:O	1:R:107:SER:HA	2.21	0.40
1:K:255:THR:O	1:K:259:ILE:HG12	2.20	0.40
1:R:114:LEU:HD23	1:R:124:GLN:HG3	2.03	0.40
1:R:79:VAL:HB	1:R:129:TYR:HB2	2.04	0.40
1:K:62:ARG:O	1:K:96:PRO:HD3	2.21	0.40
1:P:255:THR:O	1:P:259:ILE:HG12	2.21	0.40
1:E:255:THR:O	1:E:259:ILE:HG12	2.21	0.40
1:D:45:LEU:HB2	1:D:102:TYR:HB3	2.03	0.40
1:N:39:VAL:O	1:N:107:SER:HA	2.22	0.40
1:M:5:VAL:HG12	1:M:72:TRP:HA	2.02	0.40
1:Q:232:LEU:O	1:Q:236:ILE:HG12	2.21	0.40
1:D:39:VAL:O	1:D:107:SER:HA	2.22	0.40
1:D:236:ILE:CD1	1:D:263:TYR:HE1	2.35	0.40
1:R:232:LEU:O	1:R:236:ILE:HG12	2.22	0.40
1:K:306:ALA:HA	1:K:309:ILE:HD12	2.03	0.40
1:G:45:LEU:HB2	1:G:102:TYR:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:VAL:O	1:I:107:SER:HA	2.21	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	309/318 (97%)	293 (95%)	15 (5%)	1 (0%)	46 83
1	B	309/318 (97%)	290 (94%)	18 (6%)	1 (0%)	46 83
1	C	309/318 (97%)	291 (94%)	18 (6%)	0	100 100
1	D	309/318 (97%)	296 (96%)	13 (4%)	0	100 100
1	E	307/318 (96%)	290 (94%)	16 (5%)	1 (0%)	46 83
1	F	309/318 (97%)	290 (94%)	19 (6%)	0	100 100
1	G	309/318 (97%)	293 (95%)	15 (5%)	1 (0%)	46 83
1	H	305/318 (96%)	287 (94%)	18 (6%)	0	100 100
1	I	303/318 (95%)	287 (95%)	16 (5%)	0	100 100
1	J	309/318 (97%)	293 (95%)	16 (5%)	0	100 100
1	K	305/318 (96%)	289 (95%)	16 (5%)	0	100 100
1	L	298/318 (94%)	283 (95%)	15 (5%)	0	100 100
1	M	304/318 (96%)	286 (94%)	18 (6%)	0	100 100
1	N	309/318 (97%)	291 (94%)	17 (6%)	1 (0%)	46 83
1	O	309/318 (97%)	291 (94%)	18 (6%)	0	100 100
1	P	309/318 (97%)	294 (95%)	15 (5%)	0	100 100
1	Q	309/318 (97%)	290 (94%)	18 (6%)	1 (0%)	46 83
1	R	309/318 (97%)	290 (94%)	19 (6%)	0	100 100
1	S	305/318 (96%)	290 (95%)	15 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	T	309/318 (97%)	295 (96%)	14 (4%)	0	100 100
All	All	6144/6360 (97%)	5809 (94%)	329 (5%)	6 (0%)	56 90

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	6	SER
1	E	122	ASP
1	G	177	GLU
1	Q	166	THR
1	A	29	SER
1	B	25	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	230/284 (81%)	215 (94%)	15 (6%)	21 61
1	B	232/284 (82%)	220 (95%)	12 (5%)	29 67
1	C	233/284 (82%)	217 (93%)	16 (7%)	19 59
1	D	235/284 (83%)	221 (94%)	14 (6%)	24 63
1	E	239/284 (84%)	223 (93%)	16 (7%)	20 60
1	F	229/284 (81%)	216 (94%)	13 (6%)	25 65
1	G	229/284 (81%)	210 (92%)	19 (8%)	14 51
1	H	194/284 (68%)	186 (96%)	8 (4%)	37 72
1	I	181/284 (64%)	172 (95%)	9 (5%)	30 68
1	J	205/284 (72%)	193 (94%)	12 (6%)	24 63
1	K	226/284 (80%)	209 (92%)	17 (8%)	17 56
1	L	231/284 (81%)	218 (94%)	13 (6%)	26 65
1	M	217/284 (76%)	202 (93%)	15 (7%)	19 59
1	N	239/284 (84%)	222 (93%)	17 (7%)	18 58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	242/284 (85%)	230 (95%)	12 (5%)	30 68
1	P	214/284 (75%)	203 (95%)	11 (5%)	29 68
1	Q	234/284 (82%)	218 (93%)	16 (7%)	20 59
1	R	219/284 (77%)	204 (93%)	15 (7%)	20 59
1	S	214/284 (75%)	203 (95%)	11 (5%)	29 68
1	T	173/284 (61%)	167 (96%)	6 (4%)	43 76
All	All	4416/5680 (78%)	4149 (94%)	267 (6%)	24 63

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	30	LEU
1	A	31	ASP
1	A	67	GLU
1	A	85	ARG
1	A	97	ASP
1	A	107	SER
1	A	111	LEU
1	A	115	ASP
1	A	196	SER
1	A	198	ILE
1	A	248	LYS
1	A	297	ILE
1	A	305	LEU
1	A	308	ILE
1	B	24	LEU
1	B	30	LEU
1	B	31	ASP
1	B	97	ASP
1	B	107	SER
1	B	111	LEU
1	B	115	ASP
1	B	135	VAL
1	B	196	SER
1	B	198	ILE
1	B	248	LYS
1	B	312	PHE
1	C	5	VAL
1	C	24	LEU

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Mol	Chain	Res	Type
1	C	25	ILE
1	C	30	LEU
1	C	32	ASP
1	C	62	ARG
1	C	97	ASP
1	C	103	LEU
1	C	107	SER
1	C	111	LEU
1	C	115	ASP
1	C	196	SER
1	C	198	ILE
1	C	248	LYS
1	C	305	LEU
1	C	308	ILE
1	D	24	LEU
1	D	30	LEU
1	D	61	VAL
1	D	97	ASP
1	D	107	SER
1	D	111	LEU
1	D	115	ASP
1	D	139	ASN
1	D	196	SER
1	D	198	ILE
1	D	248	LYS
1	D	305	LEU
1	D	308	ILE
1	D	312	PHE
1	E	24	LEU
1	E	30	LEU
1	E	58	ARG
1	E	61	VAL
1	E	62	ARG
1	E	95	SER
1	E	107	SER
1	E	111	LEU
1	E	115	ASP
1	E	195	PHE
1	E	196	SER
1	E	198	ILE
1	E	248	LYS
1	E	293	ARG

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Mol	Chain	Res	Type
1	E	305	LEU
1	E	308	ILE
1	F	24	LEU
1	F	28	TYR
1	F	86	ASP
1	F	97	ASP
1	F	107	SER
1	F	111	LEU
1	F	115	ASP
1	F	151	LYS
1	F	188	LEU
1	F	196	SER
1	F	198	ILE
1	F	248	LYS
1	F	312	PHE
1	G	5	VAL
1	G	16	LEU
1	G	24	LEU
1	G	28	TYR
1	G	30	LEU
1	G	58	ARG
1	G	61	VAL
1	G	88	ASP
1	G	97	ASP
1	G	107	SER
1	G	111	LEU
1	G	115	ASP
1	G	133	ARG
1	G	136	ASP
1	G	196	SER
1	G	198	ILE
1	G	252	MET
1	G	305	LEU
1	G	308	ILE
1	H	58	ARG
1	H	97	ASP
1	H	111	LEU
1	H	146	LEU
1	H	196	SER
1	H	198	ILE
1	H	305	LEU
1	H	308	ILE

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Mol	Chain	Res	Type
1	I	86	ASP
1	I	97	ASP
1	I	107	SER
1	I	111	LEU
1	I	196	SER
1	I	198	ILE
1	I	248	LYS
1	I	284	GLN
1	I	308	ILE
1	J	6	SER
1	J	31	ASP
1	J	85	ARG
1	J	97	ASP
1	J	107	SER
1	J	151	LYS
1	J	196	SER
1	J	198	ILE
1	J	248	LYS
1	J	305	LEU
1	J	308	ILE
1	J	312	PHE
1	K	24	LEU
1	K	30	LEU
1	K	58	ARG
1	K	61	VAL
1	K	62	ARG
1	K	75	GLU
1	K	97	ASP
1	K	107	SER
1	K	111	LEU
1	K	115	ASP
1	K	188	LEU
1	K	195	PHE
1	K	196	SER
1	K	198	ILE
1	K	248	LYS
1	K	305	LEU
1	K	308	ILE
1	L	5	VAL
1	L	24	LEU
1	L	30	LEU
1	L	61	VAL

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Mol	Chain	Res	Type
1	L	97	ASP
1	L	107	SER
1	L	111	LEU
1	L	115	ASP
1	L	196	SER
1	L	198	ILE
1	L	248	LYS
1	L	305	LEU
1	L	308	ILE
1	M	24	LEU
1	M	25	ILE
1	M	30	LEU
1	M	31	ASP
1	M	97	ASP
1	M	107	SER
1	M	111	LEU
1	M	137	THR
1	M	196	SER
1	M	198	ILE
1	M	243	GLU
1	M	248	LYS
1	M	305	LEU
1	M	308	ILE
1	M	312	PHE
1	N	24	LEU
1	N	25	ILE
1	N	26	GLU
1	N	61	VAL
1	N	97	ASP
1	N	107	SER
1	N	111	LEU
1	N	115	ASP
1	N	151	LYS
1	N	157	LEU
1	N	188	LEU
1	N	195	PHE
1	N	196	SER
1	N	198	ILE
1	N	248	LYS
1	N	293	ARG
1	N	305	LEU
1	O	5	VAL

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Mol	Chain	Res	Type
1	O	24	LEU
1	O	25	ILE
1	O	30	LEU
1	O	61	VAL
1	O	97	ASP
1	O	107	SER
1	O	111	LEU
1	O	115	ASP
1	O	153	ASP
1	O	196	SER
1	O	305	LEU
1	P	24	LEU
1	P	30	LEU
1	P	58	ARG
1	P	97	ASP
1	P	107	SER
1	P	111	LEU
1	P	115	ASP
1	P	137	THR
1	P	196	SER
1	P	198	ILE
1	P	305	LEU
1	Q	14	GLU
1	Q	24	LEU
1	Q	30	LEU
1	Q	67	GLU
1	Q	88	ASP
1	Q	97	ASP
1	Q	107	SER
1	Q	111	LEU
1	Q	115	ASP
1	Q	195	PHE
1	Q	196	SER
1	Q	198	ILE
1	Q	248	LYS
1	Q	305	LEU
1	Q	308	ILE
1	Q	312	PHE
1	R	6	SER
1	R	30	LEU
1	R	32	ASP
1	R	86	ASP

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Mol	Chain	Res	Type
1	R	97	ASP
1	R	107	SER
1	R	111	LEU
1	R	115	ASP
1	R	157	LEU
1	R	196	SER
1	R	198	ILE
1	R	248	LYS
1	R	305	LEU
1	R	308	ILE
1	R	312	PHE
1	S	30	LEU
1	S	88	ASP
1	S	97	ASP
1	S	107	SER
1	S	111	LEU
1	S	115	ASP
1	S	196	SER
1	S	198	ILE
1	S	248	LYS
1	S	305	LEU
1	S	308	ILE
1	T	107	SER
1	T	115	ASP
1	T	196	SER
1	T	198	ILE
1	T	305	LEU
1	T	308	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	GLN
1	B	235	HIS
1	C	235	HIS
1	E	139	ASN
1	E	235	HIS
1	E	284	GLN
1	I	235	HIS
1	K	83	ASN
1	N	83	ASN
1	P	235	HIS

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Mol	Chain	Res	Type
1	Q	235	HIS
1	T	235	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	311/318 (97%)	-0.40	0 100 100	161, 244, 294, 300	0
1	B	311/318 (97%)	-0.39	1 (0%) 94 92	166, 242, 293, 300	0
1	C	311/318 (97%)	-0.42	4 (1%) 79 71	148, 226, 278, 290	0
1	D	311/318 (97%)	-0.34	2 (0%) 90 86	146, 232, 285, 295	0
1	E	311/318 (97%)	-0.45	0 100 100	145, 222, 269, 287	0
1	F	311/318 (97%)	-0.43	1 (0%) 94 92	168, 232, 285, 296	0
1	G	311/318 (97%)	-0.44	4 (1%) 79 71	174, 232, 296, 300	0
1	H	309/318 (97%)	-0.36	3 (0%) 84 77	162, 268, 300, 300	0
1	I	307/318 (96%)	-0.35	6 (1%) 68 58	178, 265, 300, 300	0
1	J	311/318 (97%)	-0.36	6 (1%) 70 61	171, 262, 300, 300	0
1	K	309/318 (97%)	-0.37	4 (1%) 79 71	163, 239, 290, 300	0
1	L	302/318 (94%)	-0.38	2 (0%) 89 84	167, 247, 290, 300	0
1	M	308/318 (96%)	-0.42	0 100 100	172, 256, 291, 299	0
1	N	311/318 (97%)	-0.43	4 (1%) 79 71	173, 255, 293, 299	0
1	O	311/318 (97%)	-0.56	0 100 100	161, 224, 278, 288	0
1	P	311/318 (97%)	-0.43	3 (0%) 84 77	168, 268, 300, 300	0
1	Q	311/318 (97%)	-0.52	1 (0%) 94 92	172, 232, 287, 300	0
1	R	311/318 (97%)	-0.39	1 (0%) 94 92	178, 239, 288, 296	0
1	S	309/318 (97%)	-0.31	5 (1%) 74 65	173, 269, 300, 300	0
1	T	311/318 (97%)	-0.08	13 (4%) 40 31	179, 270, 300, 300	0
All	All	6198/6360 (97%)	-0.39	60 (0%) 84 77	145, 245, 299, 300	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	93	SER	6.2
1	T	134	SER	5.3
1	G	153	ASP	4.0
1	J	137	THR	3.6
1	I	64	LYS	3.5
1	F	175	ALA	3.4
1	S	169	VAL	3.4
1	N	13	ASP	3.2
1	P	170	LYS	3.2
1	G	169	VAL	3.2
1	P	252	MET	3.1
1	Q	13	ASP	3.1
1	I	94	VAL	3.1
1	L	173	ASN	3.0
1	R	63	VAL	3.0
1	C	170	LYS	2.9
1	P	169	VAL	2.8
1	H	169	VAL	2.8
1	B	9	PRO	2.7
1	K	153	ASP	2.6
1	I	93	SER	2.6
1	N	153	ASP	2.5
1	J	9	PRO	2.5
1	D	97	ASP	2.5
1	D	169	VAL	2.5
1	T	60	GLY	2.5
1	J	138	ARG	2.5
1	I	11	ILE	2.5
1	K	154	ASP	2.5
1	T	136	ASP	2.4
1	S	13	ASP	2.4
1	I	250	PRO	2.4
1	T	62	ARG	2.4
1	J	139	ASN	2.3
1	T	154	ASP	2.3
1	T	169	VAL	2.3
1	T	49	ASP	2.3
1	C	61	VAL	2.2
1	J	136	ASP	2.2
1	C	83	ASN	2.2
1	H	49	ASP	2.2
1	L	83	ASN	2.2
1	S	82	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	167	ALA	2.1
1	T	99	THR	2.1
1	K	59	SER	2.1
1	I	135	VAL	2.1
1	H	50	ARG	2.1
1	N	14	GLU	2.1
1	C	153	ASP	2.1
1	T	135	VAL	2.1
1	T	34	ALA	2.1
1	G	137	THR	2.1
1	K	82	GLU	2.0
1	S	62	ARG	2.0
1	J	61	VAL	2.0
1	T	182	SER	2.0
1	T	133	ARG	2.0
1	G	154	ASP	2.0
1	N	169	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.