Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 01:12 am BST

PDB ID	:	4YEU
Title	:	ELIC-GLIC chimera in the resting conformation
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Deposited on	:	2015-02-24
Resolution	:	4.60 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 following versions of software and data (see references ⓘ) were used in the production of this report:

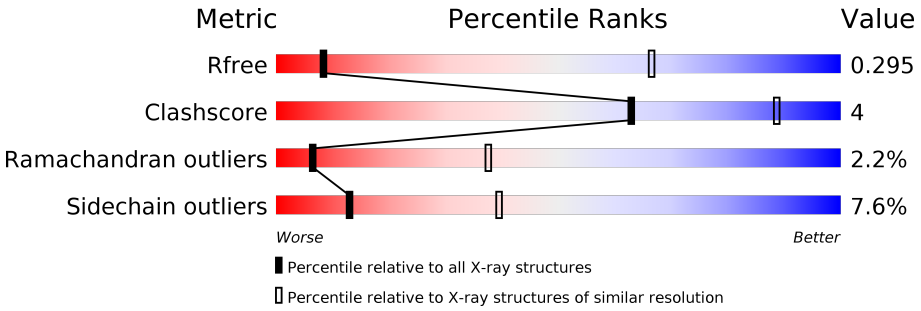
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 4.60 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}	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)

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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	312	81% 17% •
1	B	312	80% 19% •
1	C	312	80% 18% •
1	D	312	82% 16% •
1	E	312	81% 17% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12825 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 Cys-loop ligand-gated ion channel,Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2565	1686	417	457	5			
1	B	312	Total	C	N	O	S	0	0	0
			2565	1686	417	457	5			
1	C	312	Total	C	N	O	S	0	0	0
			2565	1686	417	457	5			
1	D	312	Total	C	N	O	S	0	0	0
			2565	1686	417	457	5			
1	E	312	Total	C	N	O	S	0	0	0
			2565	1686	417	457	5			

There are 5 discrepancies between the modelled and reference sequences:

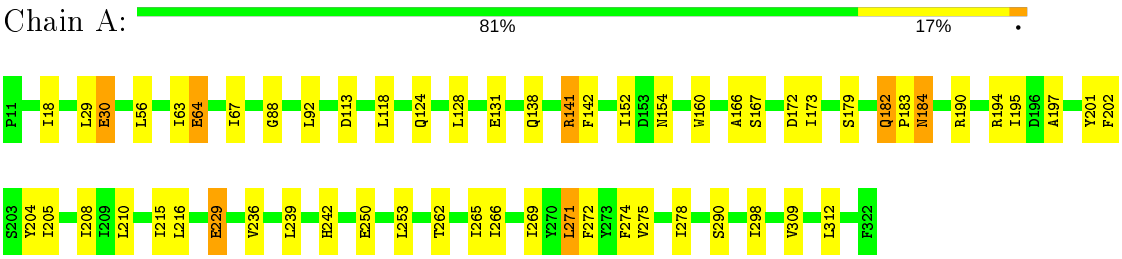
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	insertion	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
C	164	GLY	-	insertion	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

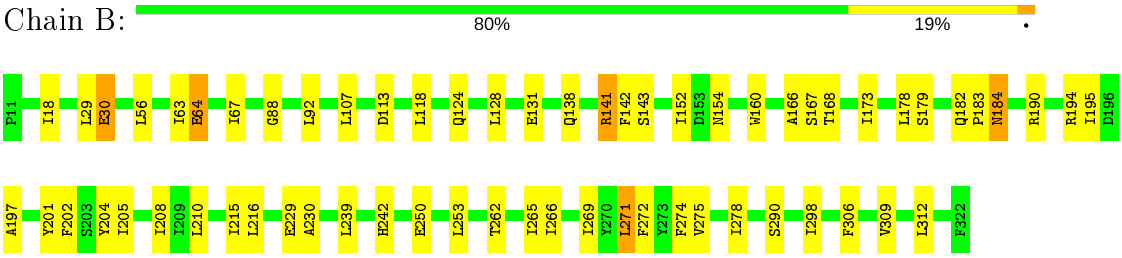
- Molecule 1: Cys-loop ligand-gated ion channel,Proton-gated ion channel

Chain A:



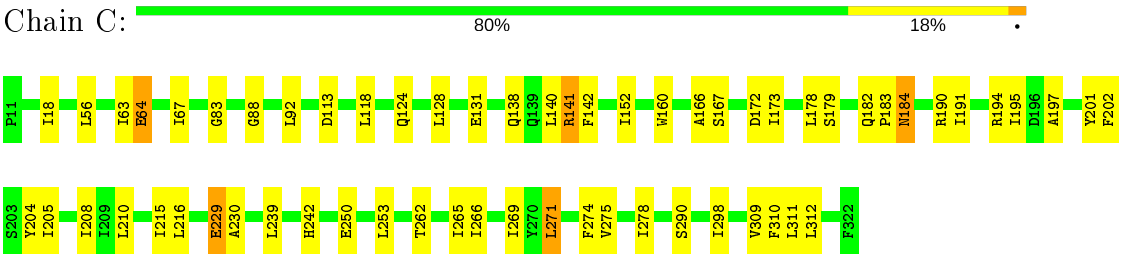
- Molecule 1: Cys-loop ligand-gated ion channel,Proton-gated ion channel

Chain B:



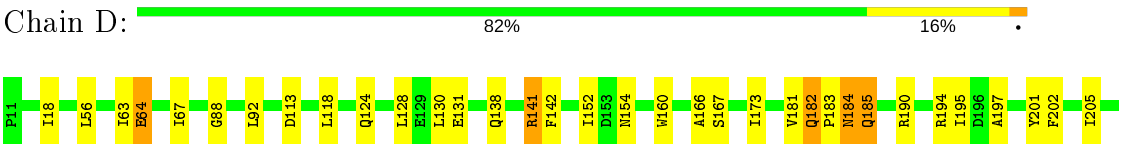
- Molecule 1: Cys-loop ligand-gated ion channel,Proton-gated ion channel

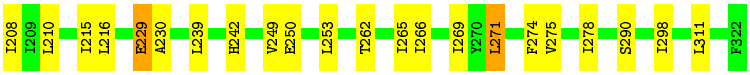
Chain C:



- Molecule 1: Cys-loop ligand-gated ion channel,Proton-gated ion channel

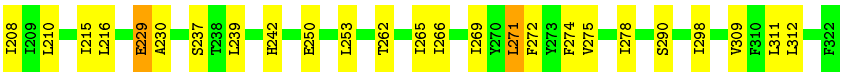
Chain D:





• Molecule 1: Cys-loop ligand-gated ion channel,Proton-gated ion channel

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	132.44Å 217.96Å 229.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.60 49.23 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-4.60) 99.3 (49.23-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 4.64Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.242 , 0.248 0.280 , 0.295	Depositor DCC
R_{free} test set	954 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	254.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 102.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.016 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	12825	wwPDB-VP
Average B, all atoms (Å^2)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, 0.333 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	0.38	0/2638	0.61	0/3600
1	B	0.38	0/2638	0.61	0/3600
1	C	0.38	0/2638	0.61	0/3600
1	D	0.38	0/2638	0.63	0/3600
1	E	0.38	0/2638	0.61	0/3600
All	All	0.38	0/13190	0.62	0/18000

There are no bond length outliers.

There are no bond angle outliers.

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	2565	0	2545	23	0
1	B	2565	0	2545	26	0
1	C	2565	0	2545	24	0
1	D	2565	0	2545	24	0
1	E	2565	0	2545	23	0
All	All	12825	0	12725	109	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 (109) 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:208:ILE:HD12	1:D:249:VAL:HG22	1.46	0.97
1:D:182:GLN:HB3	1:D:185:GLN:HB3	1.57	0.85
1:D:167:SER:HB3	1:D:194:ARG:HG3	1.71	0.73
1:E:167:SER:HB3	1:E:194:ARG:HG3	1.71	0.72
1:B:167:SER:HB3	1:B:194:ARG:HG3	1.72	0.72
1:C:167:SER:HB3	1:C:194:ARG:HG3	1.71	0.72
1:A:167:SER:HB3	1:A:194:ARG:HG3	1.71	0.70
1:D:182:GLN:HG3	1:D:184:ASN:H	1.59	0.67
1:C:215:ILE:HD12	1:C:242:HIS:HA	1.82	0.61
1:D:215:ILE:HD12	1:D:242:HIS:HA	1.82	0.61
1:A:215:ILE:HD12	1:A:242:HIS:HA	1.81	0.61
1:B:215:ILE:HD12	1:B:242:HIS:HA	1.83	0.60
1:E:215:ILE:HD12	1:E:242:HIS:HA	1.83	0.60
1:A:166:ALA:HB2	1:A:195:ILE:HG12	1.85	0.58
1:C:166:ALA:HB2	1:C:195:ILE:HG12	1.87	0.57
1:A:239:LEU:HD21	1:E:215:ILE:HG22	1.87	0.56
1:B:166:ALA:HB2	1:B:195:ILE:HG12	1.86	0.56
1:E:166:ALA:HB2	1:E:195:ILE:HG12	1.86	0.56
1:D:166:ALA:HB2	1:D:195:ILE:HG12	1.87	0.55
1:B:215:ILE:HG22	1:C:239:LEU:HD21	1.89	0.54
1:C:215:ILE:HG22	1:D:239:LEU:HD21	1.88	0.54
1:A:229:GLU:HG3	1:E:230:ALA:HB2	1.88	0.54
1:A:274:PHE:O	1:A:278:ILE:HG12	2.08	0.53
1:A:215:ILE:HG22	1:B:239:LEU:HD21	1.89	0.53
1:B:274:PHE:O	1:B:278:ILE:HG12	2.08	0.53
1:E:274:PHE:O	1:E:278:ILE:HG12	2.09	0.53
1:C:274:PHE:O	1:C:278:ILE:HG12	2.09	0.53
1:D:274:PHE:O	1:D:278:ILE:HG12	2.10	0.51
1:C:216:LEU:HD13	1:C:269:ILE:HG23	1.93	0.50
1:B:216:LEU:HD13	1:B:269:ILE:HG23	1.94	0.49
1:B:178:LEU:HD22	1:B:182:GLN:NE2	2.28	0.49
1:D:216:LEU:HD13	1:D:269:ILE:HG23	1.94	0.49
1:A:216:LEU:HD13	1:A:269:ILE:HG23	1.94	0.49
1:D:215:ILE:HG22	1:E:239:LEU:HD21	1.95	0.48
1:E:216:LEU:HD13	1:E:269:ILE:HG23	1.94	0.48
1:E:265:ILE:O	1:E:269:ILE:HG13	2.13	0.48
1:A:266:ILE:HA	1:A:269:ILE:HD12	1.95	0.48
1:B:266:ILE:HA	1:B:269:ILE:HD12	1.96	0.48
1:D:266:ILE:HA	1:D:269:ILE:HD12	1.96	0.48
1:A:265:ILE:O	1:A:269:ILE:HG13	2.14	0.47
1:B:160:TRP:HB3	1:B:197:ALA:HB1	1.96	0.47
1:C:266:ILE:HA	1:C:269:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ILE:HA	1:E:269:ILE:HD12	1.96	0.47
1:A:160:TRP:HB3	1:A:197:ALA:HB1	1.96	0.47
1:B:131:GLU:HB2	1:B:190:ARG:HG3	1.96	0.47
1:D:160:TRP:HB3	1:D:197:ALA:HB1	1.96	0.47
1:E:64:GLU:HA	1:E:67:ILE:HD12	1.97	0.47
1:E:131:GLU:HB2	1:E:190:ARG:HG3	1.97	0.47
1:C:230:ALA:HB2	1:D:229:GLU:HG3	1.97	0.47
1:D:265:ILE:O	1:D:269:ILE:HG13	2.14	0.47
1:E:160:TRP:HB3	1:E:197:ALA:HB1	1.97	0.47
1:A:131:GLU:HB2	1:A:190:ARG:HG3	1.96	0.47
1:D:131:GLU:HB2	1:D:190:ARG:HG3	1.96	0.47
1:A:64:GLU:HA	1:A:67:ILE:HD12	1.97	0.46
1:C:131:GLU:HB2	1:C:190:ARG:HG3	1.97	0.46
1:A:271:LEU:O	1:A:275:VAL:HG23	2.15	0.46
1:B:271:LEU:O	1:B:275:VAL:HG23	2.16	0.46
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.97	0.46
1:C:265:ILE:O	1:C:269:ILE:HG13	2.16	0.46
1:C:64:GLU:HA	1:C:67:ILE:HD12	1.96	0.46
1:B:265:ILE:O	1:B:269:ILE:HG13	2.14	0.46
1:C:173:ILE:HD13	1:C:190:ARG:HB3	1.97	0.46
1:E:271:LEU:O	1:E:275:VAL:HG23	2.16	0.46
1:A:182:GLN:N	1:A:183:PRO:HD3	2.31	0.46
1:A:204:TYR:HD1	1:A:208:ILE:HD12	1.80	0.46
1:D:64:GLU:HA	1:D:67:ILE:HD12	1.97	0.46
1:D:173:ILE:HD13	1:D:190:ARG:HB3	1.98	0.46
1:B:107:LEU:HD13	1:C:83:GLY:H	1.81	0.45
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.97	0.45
1:C:160:TRP:HB3	1:C:197:ALA:HB1	1.97	0.45
1:C:178:LEU:HD22	1:C:182:GLN:NE2	2.30	0.45
1:C:182:GLN:N	1:C:183:PRO:HD3	2.31	0.45
1:D:271:LEU:O	1:D:275:VAL:HG23	2.16	0.45
1:D:63:ILE:HG12	1:D:92:LEU:HD12	1.97	0.45
1:D:230:ALA:HB2	1:E:229:GLU:HG3	1.98	0.45
1:E:173:ILE:HD13	1:E:190:ARG:HB3	1.98	0.45
1:B:204:TYR:HD1	1:B:208:ILE:HD12	1.82	0.45
1:B:182:GLN:N	1:B:183:PRO:HD3	2.32	0.45
1:B:29:LEU:HD23	1:B:30:GLU:HG2	1.99	0.45
1:A:236:VAL:HG11	1:E:237:SER:HB2	1.99	0.45
1:C:271:LEU:O	1:C:275:VAL:HG23	2.18	0.44
1:B:230:ALA:HB2	1:C:229:GLU:HG3	1.99	0.44
1:A:63:ILE:HG12	1:A:92:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:TYR:HD1	1:E:208:ILE:HD12	1.81	0.44
1:B:63:ILE:HG12	1:B:92:LEU:HD12	1.99	0.44
1:D:182:GLN:HA	1:D:183:PRO:HD3	1.96	0.44
1:E:182:GLN:N	1:E:183:PRO:HD3	2.32	0.44
1:B:64:GLU:HA	1:B:67:ILE:HD12	1.98	0.44
1:B:306:PHE:HA	1:B:309:VAL:HG12	2.00	0.43
1:C:204:TYR:HD1	1:C:208:ILE:HD12	1.82	0.43
1:E:63:ILE:HG12	1:E:92:LEU:HD12	1.99	0.43
1:A:29:LEU:HD23	1:A:30:GLU:HG2	2.00	0.43
1:C:63:ILE:HG12	1:C:92:LEU:HD12	1.99	0.42
1:C:141:ARG:HE	1:C:142:PHE:HE2	1.68	0.41
1:B:272:PHE:CE2	1:B:309:VAL:HG13	2.55	0.41
1:D:141:ARG:HE	1:D:142:PHE:HE2	1.68	0.41
1:C:309:VAL:HA	1:C:312:LEU:HD12	2.03	0.41
1:D:182:GLN:CB	1:D:185:GLN:HB3	2.41	0.41
1:B:143:SER:HB3	1:B:168:THR:HG23	2.03	0.41
1:E:309:VAL:HA	1:E:312:LEU:HD12	2.03	0.41
1:D:184:ASN:HD22	1:D:184:ASN:HA	1.58	0.41
1:E:140:LEU:HD13	1:E:191:ILE:HG13	2.03	0.41
1:A:272:PHE:HZ	1:A:309:VAL:HG12	1.85	0.40
1:B:141:ARG:HE	1:B:142:PHE:HE2	1.67	0.40
1:B:309:VAL:HA	1:B:312:LEU:HD12	2.03	0.40
1:A:309:VAL:HA	1:A:312:LEU:HD12	2.03	0.40
1:A:141:ARG:HE	1:A:142:PHE:HE2	1.68	0.40
1:C:140:LEU:HD13	1:C:191:ILE:HG13	2.04	0.40
1:E:272:PHE:HZ	1:E:309:VAL:HG12	1.87	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	310/312 (99%)	278 (90%)	25 (8%)	7 (2%)	6	37
1	B	310/312 (99%)	278 (90%)	25 (8%)	7 (2%)	6	37
1	C	310/312 (99%)	278 (90%)	25 (8%)	7 (2%)	6	37
1	D	310/312 (99%)	280 (90%)	24 (8%)	6 (2%)	8	40
1	E	310/312 (99%)	278 (90%)	25 (8%)	7 (2%)	6	37
All	All	1550/1560 (99%)	1392 (90%)	124 (8%)	34 (2%)	6	37

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	GLU
1	B	250	GLU
1	C	250	GLU
1	D	250	GLU
1	E	250	GLU
1	E	141	ARG
1	A	141	ARG
1	A	202	PHE
1	A	290	SER
1	B	141	ARG
1	B	179	SER
1	B	202	PHE
1	B	290	SER
1	C	141	ARG
1	C	202	PHE
1	D	141	ARG
1	D	202	PHE
1	D	290	SER
1	E	202	PHE
1	E	290	SER
1	A	184	ASN
1	B	184	ASN
1	C	179	SER
1	C	290	SER
1	A	179	SER
1	C	184	ASN
1	E	179	SER
1	E	184	ASN
1	B	88	GLY
1	C	88	GLY
1	D	88	GLY

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Mol	Chain	Res	Type
1	E	88	GLY
1	A	88	GLY
1	D	181	VAL

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	283/283 (100%)	261 (92%)	22 (8%)	12	38
1	B	283/283 (100%)	263 (93%)	20 (7%)	14	41
1	C	283/283 (100%)	262 (93%)	21 (7%)	13	40
1	D	283/283 (100%)	260 (92%)	23 (8%)	11	37
1	E	283/283 (100%)	262 (93%)	21 (7%)	13	40
All	All	1415/1415 (100%)	1308 (92%)	107 (8%)	13	39

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	30	GLU
1	A	56	LEU
1	A	64	GLU
1	A	113	ASP
1	A	118	LEU
1	A	124	GLN
1	A	128	LEU
1	A	138	GLN
1	A	152	ILE
1	A	154	ASN
1	A	172	ASP
1	A	182	GLN
1	A	184	ASN
1	A	201	TYR
1	A	205	ILE

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Mol	Chain	Res	Type
1	A	210	LEU
1	A	229	GLU
1	A	253	LEU
1	A	262	THR
1	A	271	LEU
1	A	298	ILE
1	B	18	ILE
1	B	30	GLU
1	B	56	LEU
1	B	64	GLU
1	B	113	ASP
1	B	118	LEU
1	B	124	GLN
1	B	128	LEU
1	B	138	GLN
1	B	152	ILE
1	B	154	ASN
1	B	184	ASN
1	B	201	TYR
1	B	205	ILE
1	B	210	LEU
1	B	229	GLU
1	B	253	LEU
1	B	262	THR
1	B	271	LEU
1	B	298	ILE
1	C	18	ILE
1	C	56	LEU
1	C	64	GLU
1	C	113	ASP
1	C	118	LEU
1	C	124	GLN
1	C	128	LEU
1	C	138	GLN
1	C	152	ILE
1	C	172	ASP
1	C	184	ASN
1	C	201	TYR
1	C	205	ILE
1	C	210	LEU
1	C	229	GLU
1	C	253	LEU

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Mol	Chain	Res	Type
1	C	262	THR
1	C	271	LEU
1	C	298	ILE
1	C	310	PHE
1	C	311	LEU
1	D	18	ILE
1	D	56	LEU
1	D	64	GLU
1	D	113	ASP
1	D	118	LEU
1	D	124	GLN
1	D	128	LEU
1	D	130	LEU
1	D	138	GLN
1	D	152	ILE
1	D	154	ASN
1	D	182	GLN
1	D	184	ASN
1	D	185	GLN
1	D	201	TYR
1	D	205	ILE
1	D	210	LEU
1	D	229	GLU
1	D	253	LEU
1	D	262	THR
1	D	271	LEU
1	D	298	ILE
1	D	311	LEU
1	E	18	ILE
1	E	56	LEU
1	E	64	GLU
1	E	113	ASP
1	E	118	LEU
1	E	124	GLN
1	E	128	LEU
1	E	138	GLN
1	E	152	ILE
1	E	172	ASP
1	E	182	GLN
1	E	184	ASN
1	E	201	TYR
1	E	205	ILE

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Mol	Chain	Res	Type
1	E	210	LEU
1	E	229	GLU
1	E	253	LEU
1	E	262	THR
1	E	271	LEU
1	E	298	ILE
1	E	311	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	200	ASN
1	A	252	ASN
1	B	112	ASN
1	B	182	GLN
1	C	112	ASN
1	C	200	ASN
1	C	252	ASN
1	D	112	ASN
1	D	184	ASN
1	D	200	ASN
1	D	252	ASN
1	E	112	ASN
1	E	200	ASN
1	E	252	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.