Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:17 AM EDT

PDB ID	:	2YN6
Title	:	Pentameric Ligand-Gated Ion Channel ELIC in Complex with Barium
Authors	:	Zimmermann, I.; Marabelli, A.; Bertozzi, C.; Sivilotti, L.G.; Dutzler, R.
Deposited on	:	2012-10-12
Resolution	:	3.31 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

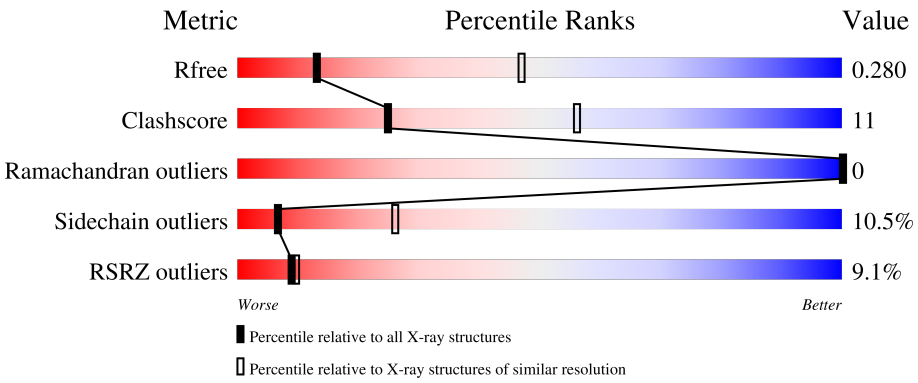
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	322	8% 69% 22% • 5%
1	B	322	10% 66% 24% 5% 5%
1	C	322	7% 64% 27% • 5%
1	D	322	9% 65% 26% • 5%
1	E	322	10% 67% 24% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12537 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 PENTAMERIC LIGAND-GATED ION CHANNEL ELIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	307	2505	1633	416	450	6	0	0	0
1	B	307	2505	1633	416	450	6	0	0	0
1	C	307	2505	1633	416	450	6	0	0	0
1	D	307	2505	1633	416	450	6	0	0	0
1	E	307	2505	1633	416	450	6	0	0	0

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba).

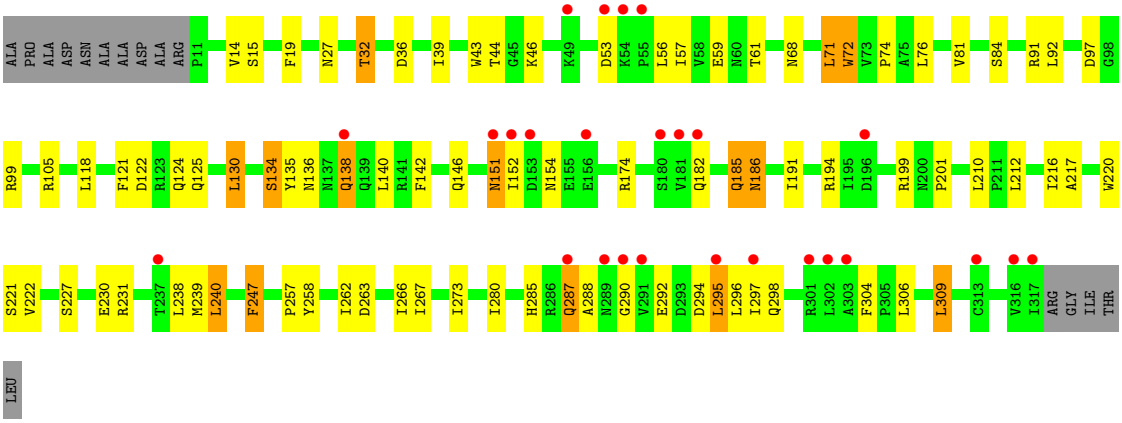
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ba		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	3	3	3	0	0
2	D	1	1	1	0	0
2	E	4	4	4	0	0

3 Residue-property plots (i)

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

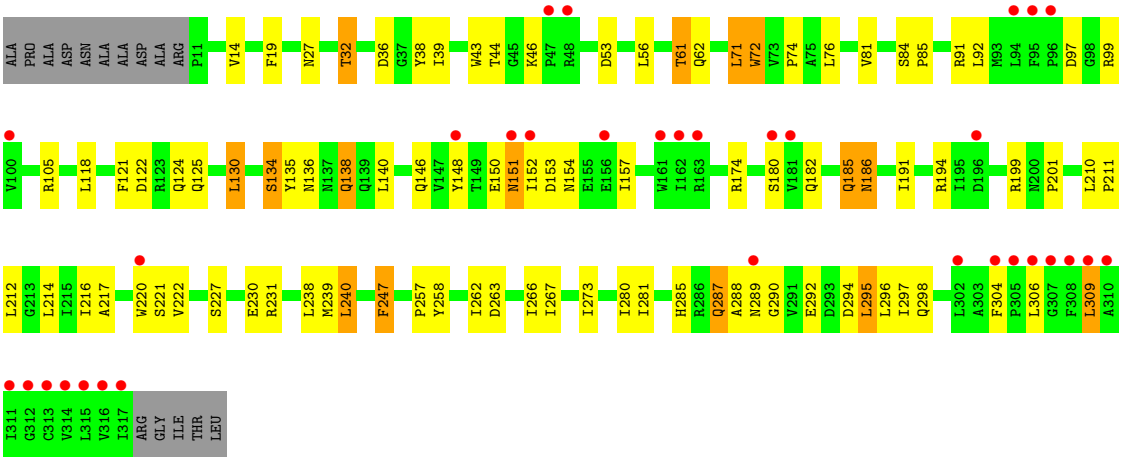
• Molecule 1: PENTAMERIC LIGAND-GATED ION CHANNEL ELIC

Chain A:



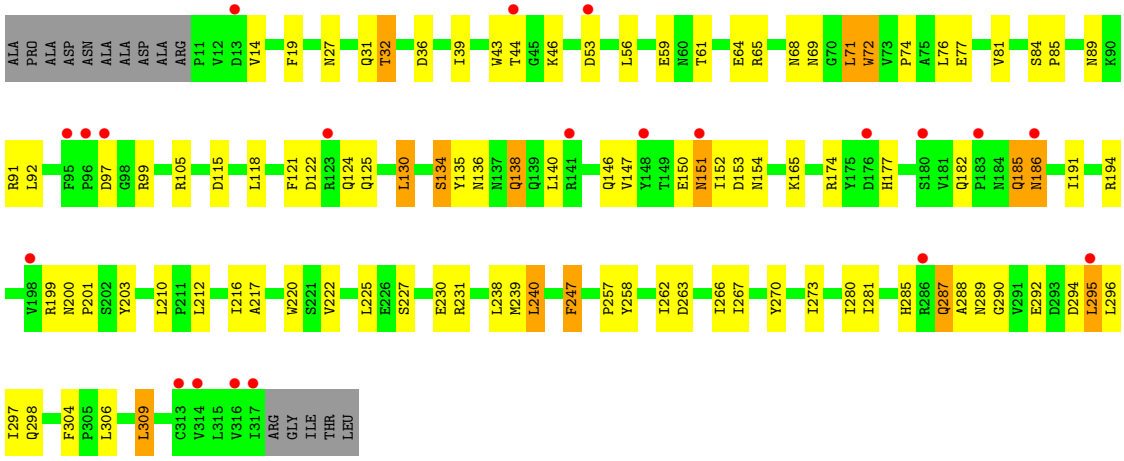
• Molecule 1: PENTAMERIC LIGAND-GATED ION CHANNEL ELIC

Chain B:



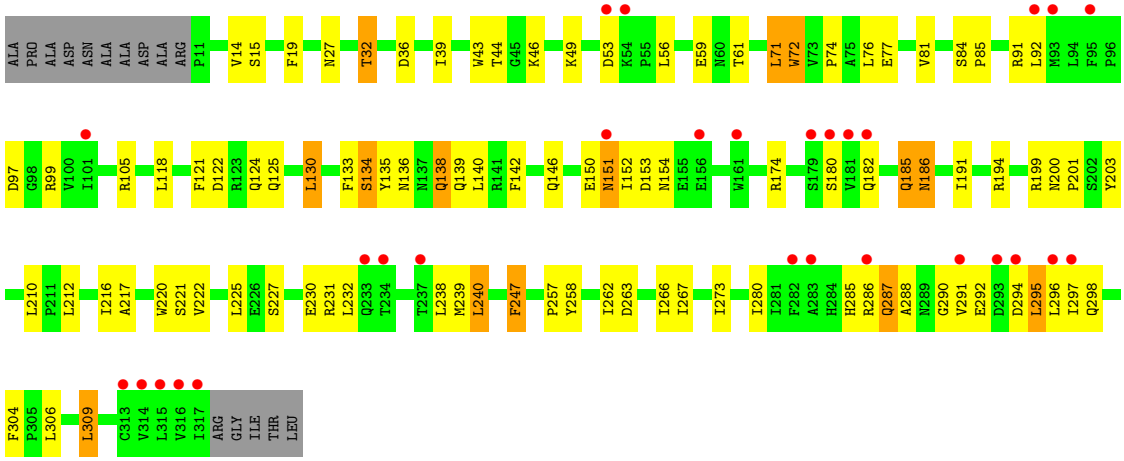
• Molecule 1: PENTAMERIC LIGAND-GATED ION CHANNEL ELIC

Chain C:



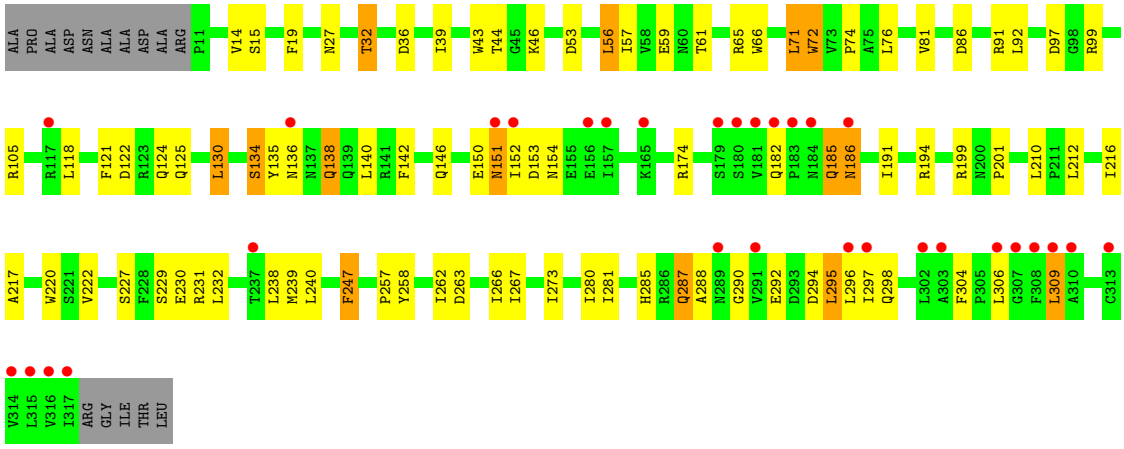
- Molecule 1: PENTAMERIC LIGAND-GATED ION CHANNEL ELIC

Chain D:



- Molecule 1: PENTAMERIC LIGAND-GATED ION CHANNEL ELIC

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	100.47Å 100.47Å 263.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.31 40.02 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.99-3.31) 99.4 (40.02-3.31)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.227 , 0.258 0.251 , 0.280	Depositor DCC
R_{free} test set	1932 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	84.3	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	12537	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BA

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	0.40	0/2573	0.61	1/3507 (0.0%)
1	B	0.40	0/2573	0.61	1/3507 (0.0%)
1	C	0.40	0/2573	0.61	1/3507 (0.0%)
1	D	0.40	0/2573	0.61	1/3507 (0.0%)
1	E	0.40	0/2573	0.61	1/3507 (0.0%)
All	All	0.40	0/12865	0.61	5/17535 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
All	All	0	10

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	GLN	N-CA-C	-6.38	93.79	111.00
1	B	138	GLN	N-CA-C	-6.38	93.79	111.00
1	D	138	GLN	N-CA-C	-6.38	93.79	111.00
1	E	138	GLN	N-CA-C	-6.37	93.80	111.00
1	C	138	GLN	N-CA-C	-6.36	93.82	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	LEU	Peptide
1	A	182	GLN	Peptide
1	B	118	LEU	Peptide
1	B	182	GLN	Peptide
1	C	118	LEU	Peptide
1	C	182	GLN	Peptide
1	D	118	LEU	Peptide
1	D	182	GLN	Peptide
1	E	118	LEU	Peptide
1	E	182	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2478	56	0
1	B	2505	0	2478	65	20
1	C	2505	0	2478	73	22
1	D	2505	0	2478	69	5
1	E	2505	0	2478	58	20
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
2	E	4	0	0	0	0
All	All	12537	0	12390	270	46

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 11.

All (270) 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:C:150:GLU:HG3	1:C:153:ASP:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLU:HG3	1:B:153:ASP:HB2	1.63	0.80
1:D:150:GLU:HG3	1:D:153:ASP:HB2	1.63	0.79
1:B:62:GLN:NE2	1:C:68:ASN:OD1	2.15	0.79
1:E:150:GLU:HG3	1:E:153:ASP:HB2	1.63	0.79
1:A:59:GLU:OE2	1:B:134:SER:OG	2.04	0.74
1:B:150:GLU:CG	1:B:153:ASP:HB2	2.19	0.73
1:C:140:LEU:HD13	1:C:191:ILE:HG13	1.71	0.73
1:C:150:GLU:CG	1:C:153:ASP:HB2	2.19	0.73
1:A:134:SER:HB3	1:E:91:ARG:HD2	1.70	0.72
1:A:140:LEU:HD13	1:A:191:ILE:HG13	1.71	0.72
1:C:247:PHE:CD2	1:D:247:PHE:HE2	2.06	0.72
1:D:140:LEU:HD13	1:D:191:ILE:HG13	1.71	0.72
1:D:150:GLU:CG	1:D:153:ASP:HB2	2.19	0.72
1:E:140:LEU:HD13	1:E:191:ILE:HG13	1.71	0.72
1:B:140:LEU:HD13	1:B:191:ILE:HG13	1.71	0.72
1:E:150:GLU:CG	1:E:153:ASP:HB2	2.19	0.72
1:C:59:GLU:OE2	1:D:134:SER:OG	2.09	0.70
1:C:91:ARG:CD	1:D:134:SER:HB3	2.24	0.68
1:A:99:ARG:HH12	1:B:180:SER:HB2	1.58	0.67
1:B:91:ARG:HD2	1:C:134:SER:HB3	1.77	0.64
1:C:91:ARG:HD2	1:D:134:SER:HB3	1.81	0.63
1:C:99:ARG:HH12	1:D:180:SER:HB2	1.62	0.63
1:B:151:ASN:OD1	1:B:151:ASN:N	2.32	0.62
1:D:151:ASN:OD1	1:D:151:ASN:N	2.32	0.62
1:C:151:ASN:N	1:C:151:ASN:OD1	2.32	0.61
1:A:151:ASN:OD1	1:A:151:ASN:N	2.32	0.60
1:E:151:ASN:N	1:E:151:ASN:OD1	2.32	0.60
1:E:257:PRO:HG2	1:E:258:TYR:CD2	2.38	0.59
1:A:257:PRO:HG2	1:A:258:TYR:CD2	2.38	0.59
1:C:105:ARG:HD3	1:D:77:GLU:OE2	2.03	0.59
1:A:247:PHE:HE2	1:E:247:PHE:CD2	2.20	0.59
1:B:257:PRO:HG2	1:B:258:TYR:CD2	2.38	0.59
1:C:257:PRO:HG2	1:C:258:TYR:CD2	2.38	0.58
1:D:227:SER:HB3	1:D:230:GLU:HG3	1.85	0.58
1:E:227:SER:HB3	1:E:230:GLU:HG3	1.86	0.58
1:D:257:PRO:HG2	1:D:258:TYR:CD2	2.38	0.58
1:C:247:PHE:CD2	1:D:247:PHE:CE2	2.90	0.58
1:B:227:SER:HB3	1:B:230:GLU:HG3	1.85	0.58
1:C:227:SER:HB3	1:C:230:GLU:HG3	1.85	0.58
1:A:294:ASP:HB2	1:A:297:ILE:HB	1.86	0.57
1:C:294:ASP:HB2	1:C:297:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:O	1:C:298:GLN:HG2	2.05	0.57
1:E:294:ASP:HB2	1:E:297:ILE:HB	1.86	0.57
1:A:227:SER:HB3	1:A:230:GLU:HG3	1.85	0.57
1:D:295:LEU:O	1:D:298:GLN:HG2	2.05	0.57
1:E:295:LEU:O	1:E:298:GLN:HG2	2.05	0.57
1:A:295:LEU:O	1:A:298:GLN:HG2	2.05	0.57
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.40	0.56
1:D:231:ARG:HB3	1:D:280:ILE:HD13	1.87	0.56
1:B:294:ASP:HB2	1:B:297:ILE:HB	1.86	0.56
1:A:19:PHE:CE2	1:A:146:GLN:HG3	2.40	0.56
1:D:294:ASP:HB2	1:D:297:ILE:HB	1.86	0.56
1:A:221:SER:HB2	1:B:281:ILE:HD11	1.87	0.56
1:C:231:ARG:HB3	1:C:280:ILE:HD13	1.88	0.56
1:B:231:ARG:HB3	1:B:280:ILE:HD13	1.87	0.56
1:B:295:LEU:O	1:B:298:GLN:HG2	2.05	0.56
1:A:231:ARG:HB3	1:A:280:ILE:HD13	1.87	0.55
1:D:71:LEU:HD22	1:D:72:TRP:H	1.72	0.55
1:A:134:SER:HB3	1:E:91:ARG:CD	2.34	0.55
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.40	0.55
1:C:71:LEU:HD22	1:C:72:TRP:H	1.71	0.55
1:C:240:LEU:HD13	1:D:240:LEU:HD11	1.89	0.55
1:E:71:LEU:HD22	1:E:72:TRP:H	1.72	0.55
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.40	0.55
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.41	0.55
1:E:231:ARG:HB3	1:E:280:ILE:HD13	1.87	0.55
1:B:186:ASN:OD1	1:B:186:ASN:N	2.40	0.55
1:D:186:ASN:N	1:D:186:ASN:OD1	2.40	0.55
1:B:71:LEU:HD22	1:B:72:TRP:H	1.72	0.54
1:D:72:TRP:CZ2	1:D:74:PRO:HG3	2.43	0.54
1:A:71:LEU:HD22	1:A:72:TRP:H	1.72	0.54
1:B:72:TRP:CZ2	1:B:74:PRO:HG3	2.43	0.54
1:A:72:TRP:CZ2	1:A:74:PRO:HG3	2.43	0.54
1:A:186:ASN:N	1:A:186:ASN:OD1	2.40	0.54
1:C:72:TRP:CZ2	1:C:74:PRO:HG3	2.43	0.54
1:B:38:TYR:OH	1:C:77:GLU:OE1	2.24	0.54
1:C:186:ASN:OD1	1:C:186:ASN:N	2.40	0.53
1:E:186:ASN:OD1	1:E:186:ASN:N	2.40	0.53
1:C:263:ASP:O	1:C:267:ILE:HG12	2.08	0.53
1:D:263:ASP:O	1:D:267:ILE:HG12	2.08	0.53
1:E:263:ASP:O	1:E:267:ILE:HG12	2.08	0.53
1:C:91:ARG:HD3	1:D:134:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:OD2	1:A:105:ARG:NH2	2.42	0.53
1:B:263:ASP:O	1:B:267:ILE:HG12	2.08	0.53
1:C:288:ALA:H	1:C:292:GLU:HB3	1.74	0.52
1:E:72:TRP:CZ2	1:E:74:PRO:HG3	2.43	0.52
1:D:288:ALA:H	1:D:292:GLU:HB3	1.74	0.52
1:A:263:ASP:O	1:A:267:ILE:HG12	2.08	0.52
1:A:288:ALA:H	1:A:292:GLU:HB3	1.74	0.52
1:C:72:TRP:CZ3	1:C:135:TYR:CZ	2.98	0.52
1:E:36:ASP:OD2	1:E:105:ARG:NH2	2.42	0.52
1:E:288:ALA:H	1:E:292:GLU:HB3	1.74	0.52
1:C:203:TYR:HB2	1:D:257:PRO:O	2.10	0.52
1:B:72:TRP:CZ3	1:B:135:TYR:CZ	2.98	0.52
1:B:288:ALA:H	1:B:292:GLU:HB3	1.74	0.51
1:B:91:ARG:CD	1:C:134:SER:HB3	2.39	0.51
1:D:72:TRP:CZ3	1:D:135:TYR:CZ	2.98	0.51
1:E:15:SER:HG	1:E:142:PHE:HE1	1.57	0.51
1:A:72:TRP:CZ3	1:A:135:TYR:CZ	2.98	0.51
1:C:247:PHE:CE2	1:D:247:PHE:HE2	2.28	0.51
1:D:36:ASP:OD2	1:D:105:ARG:NH2	2.42	0.51
1:A:91:ARG:HD2	1:B:134:SER:HB3	1.91	0.51
1:E:72:TRP:CZ3	1:E:135:TYR:CZ	2.98	0.51
1:B:150:GLU:HG3	1:B:153:ASP:CB	2.38	0.51
1:A:134:SER:HB2	1:E:57:ILE:HG21	1.93	0.50
1:A:134:SER:OG	1:E:59:GLU:OE2	2.30	0.50
1:E:150:GLU:HG3	1:E:153:ASP:CB	2.39	0.50
1:A:72:TRP:HZ3	1:A:135:TYR:CZ	2.30	0.50
1:B:36:ASP:OD2	1:B:105:ARG:NH2	2.42	0.49
1:B:214:LEU:HD12	1:C:270:TYR:HB3	1.94	0.49
1:B:72:TRP:HZ3	1:B:135:TYR:CZ	2.31	0.49
1:E:72:TRP:HZ3	1:E:135:TYR:CZ	2.30	0.49
1:C:36:ASP:OD2	1:C:105:ARG:NH2	2.42	0.49
1:C:72:TRP:HZ3	1:C:135:TYR:CZ	2.30	0.49
1:D:72:TRP:HZ3	1:D:135:TYR:CZ	2.30	0.49
1:D:91:ARG:HD2	1:E:134:SER:HB3	1.95	0.49
1:D:15:SER:HG	1:D:142:PHE:HE1	1.60	0.49
1:A:44:THR:HA	1:A:99:ARG:HA	1.96	0.48
1:D:285:HIS:C	1:D:287:GLN:HG3	2.34	0.48
1:E:285:HIS:C	1:E:287:GLN:HG3	2.34	0.48
1:C:44:THR:HA	1:C:99:ARG:HA	1.96	0.48
1:C:285:HIS:C	1:C:287:GLN:HG3	2.34	0.48
1:D:44:THR:HA	1:D:99:ARG:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:HIS:C	1:B:287:GLN:HG3	2.34	0.47
1:C:89:ASN:HB3	1:D:133:PHE:CD2	2.48	0.47
1:A:285:HIS:C	1:A:287:GLN:HG3	2.34	0.47
1:D:150:GLU:HG3	1:D:153:ASP:CB	2.39	0.47
1:E:44:THR:HA	1:E:99:ARG:HA	1.96	0.47
1:C:150:GLU:HG2	1:C:153:ASP:HB2	1.97	0.47
1:B:174:ARG:HG3	1:B:186:ASN:HB2	1.97	0.47
1:D:174:ARG:HG3	1:D:186:ASN:HB2	1.97	0.47
1:E:174:ARG:HG3	1:E:186:ASN:HB2	1.97	0.47
1:A:174:ARG:HG3	1:A:186:ASN:HB2	1.97	0.47
1:D:46:LYS:HD3	1:D:46:LYS:N	2.30	0.47
1:B:44:THR:HA	1:B:99:ARG:HA	1.96	0.46
1:A:57:ILE:HG21	1:B:134:SER:HB2	1.98	0.46
1:C:46:LYS:HD3	1:C:46:LYS:N	2.30	0.46
1:B:46:LYS:HD3	1:B:46:LYS:N	2.30	0.46
1:C:91:ARG:HH11	1:D:134:SER:HA	1.81	0.46
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.81	0.46
1:C:174:ARG:HG3	1:C:186:ASN:HB2	1.97	0.46
1:C:150:GLU:HG3	1:C:153:ASP:CB	2.38	0.46
1:C:306:LEU:HA	1:C:309:LEU:HB2	1.98	0.46
1:D:150:GLU:HG2	1:D:153:ASP:HB2	1.97	0.46
1:C:225:LEU:HD21	1:D:232:LEU:HD23	1.98	0.45
1:A:46:LYS:HD3	1:A:46:LYS:N	2.30	0.45
1:B:238:LEU:HB3	1:B:273:ILE:HD13	1.99	0.45
1:B:212:LEU:O	1:B:216:ILE:HG12	2.17	0.45
1:A:306:LEU:HA	1:A:309:LEU:HB2	1.98	0.45
1:B:136:ASN:CG	1:B:185:GLN:HB3	2.37	0.45
1:C:136:ASN:OD1	1:C:185:GLN:HB3	2.17	0.45
1:D:136:ASN:CG	1:D:185:GLN:HB3	2.37	0.45
1:E:46:LYS:HD3	1:E:46:LYS:N	2.30	0.45
1:E:306:LEU:HA	1:E:309:LEU:HB2	1.98	0.45
1:A:136:ASN:OD1	1:A:185:GLN:HB3	2.17	0.45
1:E:136:ASN:OD1	1:E:185:GLN:HB3	2.17	0.45
1:E:287:GLN:HG2	1:E:290:GLY:O	2.17	0.45
1:A:212:LEU:O	1:A:216:ILE:HG12	2.17	0.45
1:A:238:LEU:HB3	1:A:273:ILE:HD13	1.99	0.45
1:C:136:ASN:CG	1:C:185:GLN:HB3	2.37	0.45
1:C:212:LEU:O	1:C:216:ILE:HG12	2.17	0.45
1:D:212:LEU:O	1:D:216:ILE:HG12	2.17	0.45
1:D:287:GLN:HG2	1:D:290:GLY:O	2.17	0.45
1:B:221:SER:HB2	1:C:281:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LEU:HA	1:B:309:LEU:HB2	1.98	0.45
1:C:287:GLN:HG2	1:C:290:GLY:O	2.17	0.45
1:D:238:LEU:HB3	1:D:273:ILE:HD13	1.99	0.45
1:E:136:ASN:CG	1:E:185:GLN:HB3	2.37	0.45
1:E:150:GLU:HG2	1:E:153:ASP:HB2	1.97	0.45
1:A:91:ARG:CD	1:B:134:SER:HB3	2.47	0.45
1:A:247:PHE:HE2	1:E:247:PHE:CE2	2.34	0.44
1:D:203:TYR:HB2	1:E:257:PRO:O	2.18	0.44
1:A:136:ASN:CG	1:A:185:GLN:HB3	2.37	0.44
1:C:238:LEU:HB3	1:C:273:ILE:HD13	1.99	0.44
1:D:306:LEU:HA	1:D:309:LEU:HB2	1.98	0.44
1:D:221:SER:HB2	1:E:281:ILE:HD11	2.00	0.44
1:B:287:GLN:HG2	1:B:290:GLY:O	2.17	0.44
1:E:212:LEU:O	1:E:216:ILE:HG12	2.17	0.44
1:D:136:ASN:OD1	1:D:185:GLN:HB3	2.17	0.44
1:A:14:VAL:HG22	1:A:43:TRP:HB3	2.00	0.44
1:A:15:SER:HG	1:A:142:PHE:HE1	1.64	0.44
1:B:84:SER:HA	1:B:85:PRO:HD3	1.85	0.44
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.81	0.44
1:D:59:GLU:OE2	1:E:134:SER:OG	2.36	0.44
1:B:14:VAL:HG22	1:B:43:TRP:HB3	2.00	0.44
1:B:76:LEU:HB3	1:B:130:LEU:HD21	2.00	0.44
1:C:76:LEU:HB3	1:C:130:LEU:HD21	2.00	0.44
1:C:200:ASN:HA	1:C:201:PRO:HD3	1.85	0.44
1:A:76:LEU:HB3	1:A:130:LEU:HD21	2.00	0.43
1:A:287:GLN:HG2	1:A:290:GLY:O	2.17	0.43
1:D:76:LEU:HB3	1:D:130:LEU:HD21	2.00	0.43
1:A:247:PHE:CD2	1:B:247:PHE:HE2	2.36	0.43
1:B:136:ASN:OD1	1:B:185:GLN:HB3	2.17	0.43
1:C:14:VAL:HG22	1:C:43:TRP:HB3	2.00	0.43
1:C:199:ARG:O	1:C:201:PRO:HD3	2.19	0.43
1:D:14:VAL:HG22	1:D:43:TRP:HB3	2.00	0.43
1:E:14:VAL:HG22	1:E:43:TRP:HB3	2.00	0.43
1:C:247:PHE:CE2	1:D:247:PHE:CE2	3.07	0.43
1:E:199:ARG:O	1:E:201:PRO:HD3	2.19	0.43
1:E:238:LEU:HB3	1:E:273:ILE:HD13	1.99	0.43
1:A:262:ILE:O	1:A:266:ILE:HG12	2.19	0.43
1:E:76:LEU:HB3	1:E:130:LEU:HD21	2.00	0.43
1:E:92:LEU:HA	1:E:92:LEU:HD23	1.81	0.43
1:A:84:SER:OG	1:E:86:ASP:OD1	2.31	0.43
1:B:150:GLU:HG2	1:B:153:ASP:HB2	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.80	0.43
1:B:262:ILE:O	1:B:266:ILE:HG12	2.19	0.43
1:D:27:ASN:HB3	1:D:32:THR:HG22	2.01	0.43
1:A:199:ARG:O	1:A:201:PRO:HD3	2.19	0.43
1:B:148:TYR:HH	1:C:177:HIS:CE1	2.34	0.43
1:D:199:ARG:O	1:D:201:PRO:HD3	2.19	0.43
1:D:232:LEU:HA	1:D:232:LEU:HD12	1.84	0.43
1:A:27:ASN:HB3	1:A:32:THR:HG22	2.01	0.42
1:A:247:PHE:CE2	1:B:247:PHE:HE2	2.37	0.42
1:B:27:ASN:HB3	1:B:32:THR:HG22	2.01	0.42
1:B:199:ARG:O	1:B:201:PRO:HD3	2.19	0.42
1:E:217:ALA:HA	1:E:220:TRP:CE3	2.54	0.42
1:A:217:ALA:HA	1:A:220:TRP:CE3	2.54	0.42
1:E:262:ILE:O	1:E:266:ILE:HG12	2.19	0.42
1:A:68:ASN:ND2	1:E:65:ARG:HD2	2.34	0.42
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.81	0.42
1:B:150:GLU:HG2	1:B:150:GLU:O	2.20	0.42
1:C:14:VAL:HG21	1:C:138:GLN:NE2	2.35	0.42
1:C:27:ASN:HB3	1:C:32:THR:HG22	2.01	0.42
1:D:262:ILE:O	1:D:266:ILE:HG12	2.19	0.42
1:A:14:VAL:HG21	1:A:138:GLN:NE2	2.35	0.42
1:D:217:ALA:HA	1:D:220:TRP:CE3	2.54	0.42
1:C:217:ALA:HA	1:C:220:TRP:CE3	2.54	0.42
1:C:262:ILE:O	1:C:266:ILE:HG12	2.19	0.42
1:A:240:LEU:HD13	1:B:240:LEU:HD11	2.01	0.42
1:B:217:ALA:HA	1:B:220:TRP:CE3	2.54	0.42
1:E:232:LEU:HD12	1:E:232:LEU:HA	1.84	0.42
1:D:14:VAL:HG21	1:D:138:GLN:NE2	2.35	0.42
1:B:14:VAL:HG21	1:B:138:GLN:NE2	2.35	0.42
1:B:157:ILE:HD11	1:C:115:ASP:OD2	2.20	0.42
1:D:39:ILE:HD11	1:D:130:LEU:HD11	2.02	0.42
1:B:39:ILE:HD11	1:B:130:LEU:HD11	2.02	0.42
1:B:294:ASP:CB	1:B:297:ILE:HB	2.50	0.42
1:C:150:GLU:HG2	1:C:150:GLU:O	2.20	0.42
1:B:61:THR:HG21	1:C:64:GLU:CD	2.40	0.41
1:D:84:SER:HA	1:D:85:PRO:HD3	1.86	0.41
1:D:309:LEU:HD12	1:D:309:LEU:HA	1.81	0.41
1:A:39:ILE:HD11	1:A:130:LEU:HD11	2.02	0.41
1:A:294:ASP:CB	1:A:297:ILE:HB	2.50	0.41
1:D:91:ARG:CD	1:E:134:SER:HB3	2.50	0.41
1:C:147:VAL:HG12	1:C:165:LYS:HZ2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ILE:HD11	1:E:130:LEU:HD11	2.02	0.41
1:B:211:PRO:HB3	1:C:270:TYR:CD2	2.56	0.41
1:C:84:SER:HA	1:C:85:PRO:HD3	1.85	0.41
1:E:14:VAL:HG21	1:E:138:GLN:NE2	2.35	0.41
1:E:27:ASN:HB3	1:E:32:THR:HG22	2.01	0.41
1:E:294:ASP:CB	1:E:297:ILE:HB	2.50	0.41
1:C:97:ASP:OD2	1:C:99:ARG:HG2	2.21	0.41
1:E:150:GLU:HG2	1:E:150:GLU:O	2.21	0.41
1:B:97:ASP:OD2	1:B:99:ARG:HG2	2.21	0.41
1:D:225:LEU:HD21	1:E:232:LEU:HD23	2.02	0.41
1:D:286:ARG:HA	1:D:286:ARG:HD3	1.86	0.41
1:B:157:ILE:HG22	1:C:31:GLN:HE22	1.86	0.40
1:E:97:ASP:OD2	1:E:99:ARG:HG2	2.21	0.40
1:A:97:ASP:OD2	1:A:99:ARG:HG2	2.21	0.40
1:B:247:PHE:CD2	1:C:247:PHE:HE2	2.39	0.40
1:C:238:LEU:HD13	1:C:238:LEU:HA	1.96	0.40
1:D:97:ASP:OD2	1:D:99:ARG:HG2	2.21	0.40
1:A:309:LEU:HA	1:A:309:LEU:HD12	1.81	0.40
1:C:225:LEU:CD2	1:D:232:LEU:HD23	2.51	0.40
1:D:92:LEU:HA	1:D:92:LEU:HD23	1.81	0.40
1:D:150:GLU:HG2	1:D:150:GLU:O	2.20	0.40
1:C:39:ILE:HD11	1:C:130:LEU:HD11	2.02	0.40
1:D:200:ASN:HA	1:D:201:PRO:HD3	1.85	0.40

All (46) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ASN:OD1	1:E:66:TRP:CE2[1_545]	0.86	1.34
1:B:289:ASN:CG	1:E:66:TRP:CZ2[1_545]	0.95	1.25
1:B:289:ASN:CG	1:E:66:TRP:CE2[1_545]	0.96	1.24
1:B:289:ASN:OD1	1:E:66:TRP:CZ2[1_545]	1.05	1.15
1:C:69:ASN:ND2	1:C:288:ALA:N[1_565]	1.36	0.84
1:C:65:ARG:NE	1:C:289:ASN:OD1[1_565]	1.43	0.77
1:B:289:ASN:ND2	1:E:66:TRP:CD2[1_545]	1.45	0.75
1:C:69:ASN:OD1	1:C:287:GLN:O[1_565]	1.45	0.75
1:B:289:ASN:ND2	1:E:66:TRP:CE2[1_545]	1.49	0.71
1:C:69:ASN:OD1	1:C:287:GLN:C[1_565]	1.49	0.71
1:C:69:ASN:OD1	1:C:288:ALA:N[1_565]	1.51	0.69
1:C:69:ASN:CG	1:C:288:ALA:N[1_565]	1.51	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLY:N	1:E:66:TRP:CH2[1_545]	1.59	0.61
1:C:69:ASN:OD1	1:C:288:ALA:CA[1_565]	1.61	0.59
1:B:289:ASN:CB	1:E:66:TRP:CZ2[1_545]	1.64	0.56
1:B:289:ASN:OD1	1:E:66:TRP:NE1[1_545]	1.68	0.52
1:C:69:ASN:ND2	1:C:292:GLU:OE1[1_565]	1.68	0.52
1:D:46:LYS:CD	1:D:291:VAL:CG2[1_565]	1.71	0.49
1:C:65:ARG:O	1:C:288:ALA:CA[1_565]	1.75	0.45
1:C:69:ASN:CG	1:C:288:ALA:CA[1_565]	1.77	0.43
1:C:65:ARG:O	1:C:288:ALA:C[1_565]	1.80	0.40
1:C:65:ARG:O	1:C:288:ALA:CB[1_565]	1.86	0.34
1:C:69:ASN:CG	1:C:287:GLN:C[1_565]	1.87	0.33
1:B:289:ASN:O	1:E:56:LEU:CD1[1_545]	1.89	0.31
1:B:289:ASN:CG	1:E:66:TRP:CH2[1_545]	1.92	0.28
1:B:289:ASN:CA	1:E:56:LEU:CD1[1_545]	1.94	0.26
1:D:46:LYS:CE	1:D:291:VAL:CG2[1_565]	1.99	0.21
1:B:289:ASN:CG	1:E:66:TRP:NE1[1_545]	2.00	0.20
1:B:289:ASN:CG	1:E:66:TRP:CD2[1_545]	2.00	0.20
1:C:68:ASN:CB	1:C:288:ALA:O[1_565]	2.00	0.20
1:C:69:ASN:OD1	1:C:288:ALA:C[1_565]	2.01	0.19
1:C:65:ARG:NH2	1:C:292:GLU:N[1_565]	2.04	0.16
1:C:65:ARG:CG	1:C:289:ASN:CG[1_565]	2.05	0.15
1:B:289:ASN:CA	1:E:66:TRP:CZ2[1_545]	2.06	0.14
1:C:69:ASN:ND2	1:C:288:ALA:CA[1_565]	2.06	0.14
1:B:289:ASN:ND2	1:E:66:TRP:CE3[1_545]	2.07	0.13
1:D:46:LYS:CD	1:D:291:VAL:CB[1_565]	2.09	0.11
1:C:65:ARG:CG	1:C:289:ASN:ND2[1_565]	2.11	0.09
1:B:289:ASN:OD1	1:E:66:TRP:CD2[1_545]	2.12	0.08
1:B:289:ASN:C	1:E:56:LEU:CD1[1_545]	2.12	0.08
1:C:65:ARG:CD	1:C:289:ASN:ND2[1_565]	2.12	0.08
1:D:49:LYS:NZ	1:E:229:SER:OG[1_565]	2.14	0.06
1:C:65:ARG:C	1:C:288:ALA:CB[1_565]	2.15	0.05
1:B:289:ASN:ND2	1:E:66:TRP:CZ2[1_545]	2.16	0.04
1:C:65:ARG:CD	1:C:289:ASN:OD1[1_565]	2.16	0.04
1:B:174:ARG:NH2	1:D:139:GLN:OE1[3_554]	2.19	0.01

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	305/322 (95%)	287 (94%)	18 (6%)	0	100	100
1	B	305/322 (95%)	287 (94%)	18 (6%)	0	100	100
1	C	305/322 (95%)	287 (94%)	18 (6%)	0	100	100
1	D	305/322 (95%)	287 (94%)	18 (6%)	0	100	100
1	E	305/322 (95%)	286 (94%)	19 (6%)	0	100	100
All	All	1525/1610 (95%)	1434 (94%)	91 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	275/284 (97%)	246 (90%)	29 (10%)	7	26
1	B	275/284 (97%)	246 (90%)	29 (10%)	7	26
1	C	275/284 (97%)	246 (90%)	29 (10%)	7	26
1	D	275/284 (97%)	246 (90%)	29 (10%)	7	26
1	E	275/284 (97%)	246 (90%)	29 (10%)	7	26
All	All	1375/1420 (97%)	1230 (90%)	145 (10%)	7	26

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	53	ASP
1	A	56	LEU
1	A	61	THR
1	A	71	LEU
1	A	72	TRP

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Mol	Chain	Res	Type
1	A	81	VAL
1	A	121	PHE
1	A	122	ASP
1	A	124	GLN
1	A	125	GLN
1	A	130	LEU
1	A	134	SER
1	A	151	ASN
1	A	152	ILE
1	A	154	ASN
1	A	185	GLN
1	A	186	ASN
1	A	194	ARG
1	A	210	LEU
1	A	222	VAL
1	A	239	MET
1	A	240	LEU
1	A	247	PHE
1	A	287	GLN
1	A	295	LEU
1	A	296	LEU
1	A	304	PHE
1	A	309	LEU
1	B	32	THR
1	B	53	ASP
1	B	56	LEU
1	B	61	THR
1	B	71	LEU
1	B	72	TRP
1	B	81	VAL
1	B	121	PHE
1	B	122	ASP
1	B	124	GLN
1	B	125	GLN
1	B	130	LEU
1	B	134	SER
1	B	151	ASN
1	B	152	ILE
1	B	154	ASN
1	B	185	GLN
1	B	186	ASN
1	B	194	ARG

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Mol	Chain	Res	Type
1	B	210	LEU
1	B	222	VAL
1	B	239	MET
1	B	240	LEU
1	B	247	PHE
1	B	287	GLN
1	B	295	LEU
1	B	296	LEU
1	B	304	PHE
1	B	309	LEU
1	C	32	THR
1	C	53	ASP
1	C	56	LEU
1	C	61	THR
1	C	71	LEU
1	C	72	TRP
1	C	81	VAL
1	C	121	PHE
1	C	122	ASP
1	C	124	GLN
1	C	125	GLN
1	C	130	LEU
1	C	134	SER
1	C	151	ASN
1	C	152	ILE
1	C	154	ASN
1	C	185	GLN
1	C	186	ASN
1	C	194	ARG
1	C	210	LEU
1	C	222	VAL
1	C	239	MET
1	C	240	LEU
1	C	247	PHE
1	C	287	GLN
1	C	295	LEU
1	C	296	LEU
1	C	304	PHE
1	C	309	LEU
1	D	32	THR
1	D	53	ASP
1	D	56	LEU

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Mol	Chain	Res	Type
1	D	61	THR
1	D	71	LEU
1	D	72	TRP
1	D	81	VAL
1	D	121	PHE
1	D	122	ASP
1	D	124	GLN
1	D	125	GLN
1	D	130	LEU
1	D	134	SER
1	D	151	ASN
1	D	152	ILE
1	D	154	ASN
1	D	185	GLN
1	D	186	ASN
1	D	194	ARG
1	D	210	LEU
1	D	222	VAL
1	D	239	MET
1	D	240	LEU
1	D	247	PHE
1	D	287	GLN
1	D	295	LEU
1	D	296	LEU
1	D	304	PHE
1	D	309	LEU
1	E	32	THR
1	E	53	ASP
1	E	56	LEU
1	E	61	THR
1	E	71	LEU
1	E	72	TRP
1	E	81	VAL
1	E	121	PHE
1	E	122	ASP
1	E	124	GLN
1	E	125	GLN
1	E	130	LEU
1	E	134	SER
1	E	151	ASN
1	E	152	ILE
1	E	154	ASN

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Mol	Chain	Res	Type
1	E	185	GLN
1	E	186	ASN
1	E	194	ARG
1	E	210	LEU
1	E	222	VAL
1	E	239	MET
1	E	240	LEU
1	E	247	PHE
1	E	287	GLN
1	E	295	LEU
1	E	296	LEU
1	E	304	PHE
1	E	309	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	B	103	ASN
1	C	31	GLN
1	D	103	ASN
1	E	103	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	307/322 (95%)	0.52	26 (8%)	10	11	44, 79, 175, 353	0
1	B	307/322 (95%)	0.52	33 (10%)	6	5	41, 75, 200, 509	0
1	C	307/322 (95%)	0.35	21 (6%)	17	18	39, 72, 176, 550	0
1	D	307/322 (95%)	0.47	29 (9%)	8	9	34, 70, 194, 304	0
1	E	307/322 (95%)	0.45	31 (10%)	7	7	46, 78, 194, 276	0
All	All	1535/1610 (95%)	0.46	140 (9%)	9	10	34, 75, 193, 550	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	SER	10.7
1	E	180	SER	9.2
1	B	313	CYS	8.9
1	D	316	VAL	7.3
1	D	317	ILE	7.0
1	B	312	GLY	6.8
1	B	314	VAL	6.8
1	E	306	LEU	6.6
1	B	308	PHE	6.4
1	B	306	LEU	6.3
1	E	181	VAL	6.3
1	D	296	LEU	6.2
1	A	290	GLY	6.0
1	E	179	SER	5.9
1	D	315	LEU	5.9
1	B	305	PRO	5.8
1	E	317	ILE	5.4
1	D	180	SER	5.3
1	A	156	GLU	5.2
1	E	313	CYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	153	ASP	5.1
1	B	151	ASN	5.1
1	B	316	VAL	4.9
1	D	313	CYS	4.9
1	D	297	ILE	4.8
1	B	315	LEU	4.8
1	B	310	ALA	4.8
1	B	302	LEU	4.7
1	B	309	LEU	4.6
1	E	310	ALA	4.6
1	B	311	ILE	4.4
1	E	291	VAL	4.3
1	B	289	ASN	4.3
1	E	316	VAL	4.3
1	B	307	GLY	4.3
1	A	53	ASP	4.2
1	A	291	VAL	4.0
1	A	302	LEU	4.0
1	E	152	ILE	4.0
1	A	196	ASP	4.0
1	E	156	GLU	3.9
1	C	317	ILE	3.9
1	D	179	SER	3.8
1	D	181	VAL	3.7
1	B	304	PHE	3.7
1	B	161	TRP	3.5
1	A	151	ASN	3.5
1	B	48	ARG	3.5
1	A	289	ASN	3.5
1	C	97	ASP	3.4
1	A	313	CYS	3.4
1	C	96	PRO	3.4
1	E	314	VAL	3.3
1	B	317	ILE	3.3
1	D	156	GLU	3.3
1	E	307	GLY	3.3
1	E	151	ASN	3.2
1	A	152	ILE	3.2
1	A	295	LEU	3.1
1	E	296	LEU	3.1
1	B	152	ILE	3.1
1	E	157	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	182	GLN	3.0
1	C	141	ARG	3.0
1	A	317	ILE	3.0
1	D	314	VAL	3.0
1	C	53	ASP	3.0
1	E	237	THR	3.0
1	E	183	PRO	3.0
1	D	95	PHE	2.8
1	D	282	PHE	2.8
1	D	237	THR	2.8
1	A	181	VAL	2.8
1	A	287	GLN	2.8
1	C	316	VAL	2.8
1	B	163	ARG	2.7
1	A	180	SER	2.7
1	D	53	ASP	2.7
1	B	96	PRO	2.7
1	E	309	LEU	2.7
1	E	308	PHE	2.6
1	B	100	VAL	2.6
1	E	297	ILE	2.5
1	C	13	ASP	2.5
1	D	294	ASP	2.5
1	B	156	GLU	2.5
1	C	313	CYS	2.5
1	E	302	LEU	2.5
1	B	220	TRP	2.4
1	D	234	THR	2.4
1	A	237	THR	2.4
1	B	196	ASP	2.3
1	C	176	ASP	2.3
1	D	291	VAL	2.3
1	A	55	PRO	2.3
1	C	186	ASN	2.3
1	D	182	GLN	2.3
1	A	303	ALA	2.3
1	C	123	ARG	2.3
1	C	148	TYR	2.3
1	A	301	ARG	2.3
1	D	233	GLN	2.3
1	E	184	ASN	2.2
1	C	180	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	303	ALA	2.2
1	C	295	LEU	2.2
1	C	314	VAL	2.2
1	A	316	VAL	2.2
1	B	181	VAL	2.2
1	E	182	GLN	2.2
1	D	286	ARG	2.2
1	B	94	LEU	2.2
1	D	93	MET	2.2
1	E	165	LYS	2.2
1	D	54	LYS	2.1
1	D	161	TRP	2.1
1	A	54	LYS	2.1
1	D	151	ASN	2.1
1	C	44	THR	2.1
1	B	162	ILE	2.1
1	C	286	ARG	2.1
1	C	183	PRO	2.1
1	D	293	ASP	2.1
1	B	95	PHE	2.1
1	E	186	ASN	2.1
1	A	49	LYS	2.1
1	A	297	ILE	2.1
1	D	92	LEU	2.1
1	E	315	LEU	2.1
1	C	95	PHE	2.1
1	B	47	PRO	2.1
1	E	136	ASN	2.0
1	E	117	ARG	2.0
1	B	148	TYR	2.0
1	C	198	VAL	2.0
1	D	283	ALA	2.0
1	C	151	ASN	2.0
1	D	101	ILE	2.0
1	E	289	ASN	2.0
1	A	138	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BA	C	1320	1/1	0.51	0.23	256,256,256,256	0
2	BA	B	1318	1/1	0.55	0.16	216,216,216,216	0
2	BA	A	1319	1/1	0.57	0.14	203,203,203,203	0
2	BA	C	1319	1/1	0.58	0.10	237,237,237,237	0
2	BA	A	1318	1/1	0.59	0.10	227,227,227,227	0
2	BA	E	1318	1/1	0.63	0.08	258,258,258,258	0
2	BA	E	1320	1/1	0.67	0.12	222,222,222,222	0
2	BA	D	1318	1/1	0.71	0.16	224,224,224,224	0
2	BA	E	1319	1/1	0.74	0.22	259,259,259,259	0
2	BA	C	1318	1/1	0.75	0.08	211,211,211,211	0
2	BA	E	1321	1/1	0.86	0.15	200,200,200,200	0
2	BA	B	1319	1/1	0.92	0.23	229,229,229,229	0

6.5 Other polymers (i)

There are no such residues in this entry.