



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:09 PM EDT

PDB ID : 2WJX / pdb_00002wjx
Title : Crystal structure of the human ionotropic glutamate receptor GluR2 ATD region at 4.1 Å resolution
Authors : Clayton, A.; Siebold, C.; Gilbert, R.J.C.; Sutton, G.C.; Harlos, K.; McIlhinney, R.A.J.; Jones, E.Y.; Aricescu, A.R.
Deposited on : 2009-06-01
Resolution : 4.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

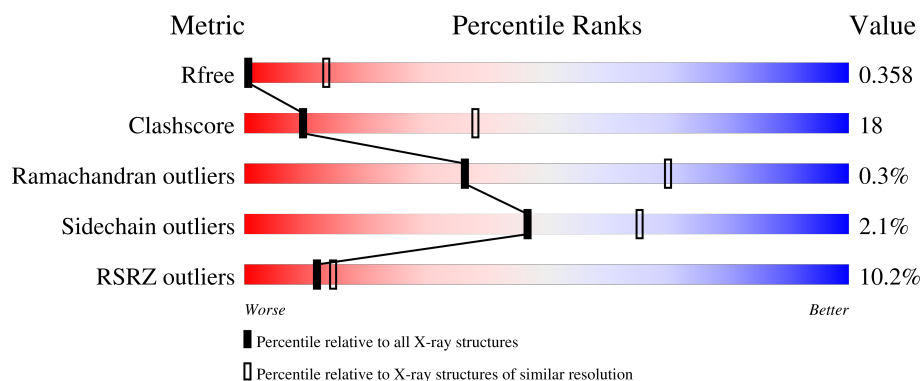
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	388	9% 66% 24% 6%
1	B	388	11% 69% 22% 6%
1	C	388	8% 71% 20% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8706 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.

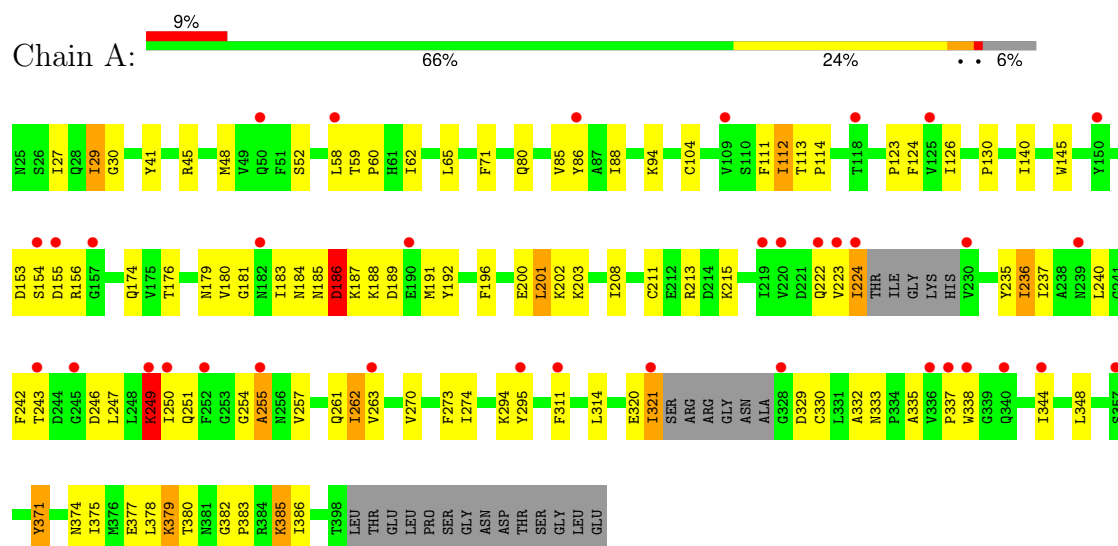
- Molecule 1 is a protein called GLUTAMATE RECEPTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2902	1852	489	551	10			
1	B	363	Total	C	N	O	S	0	0	0
			2902	1852	489	551	10			
1	C	363	Total	C	N	O	S	0	0	0
			2902	1852	489	551	10			

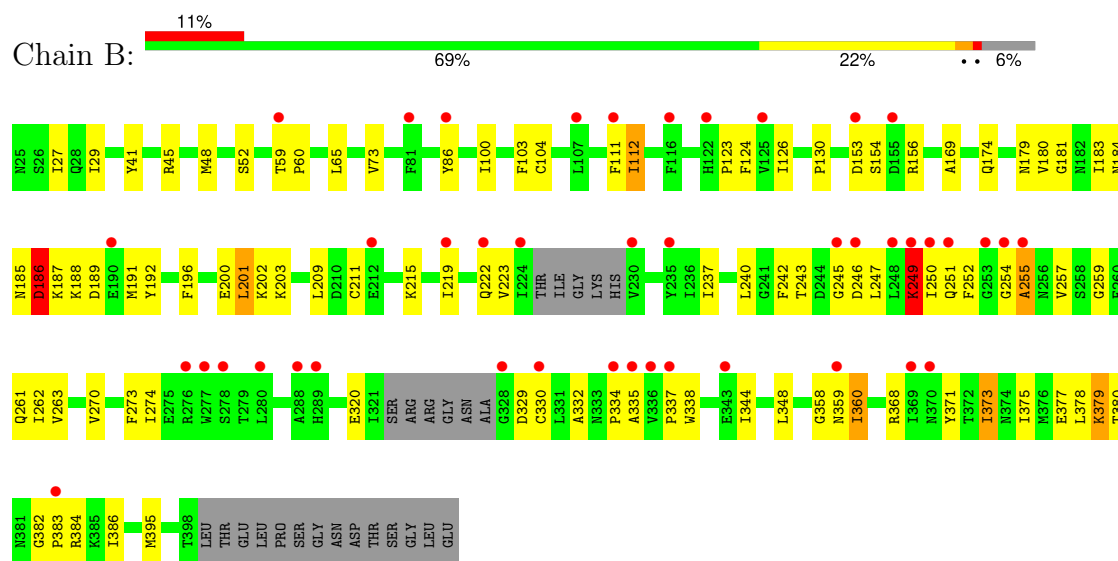
3 Residue-property plots [i](#)

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: GLUTAMATE RECEPTOR 2

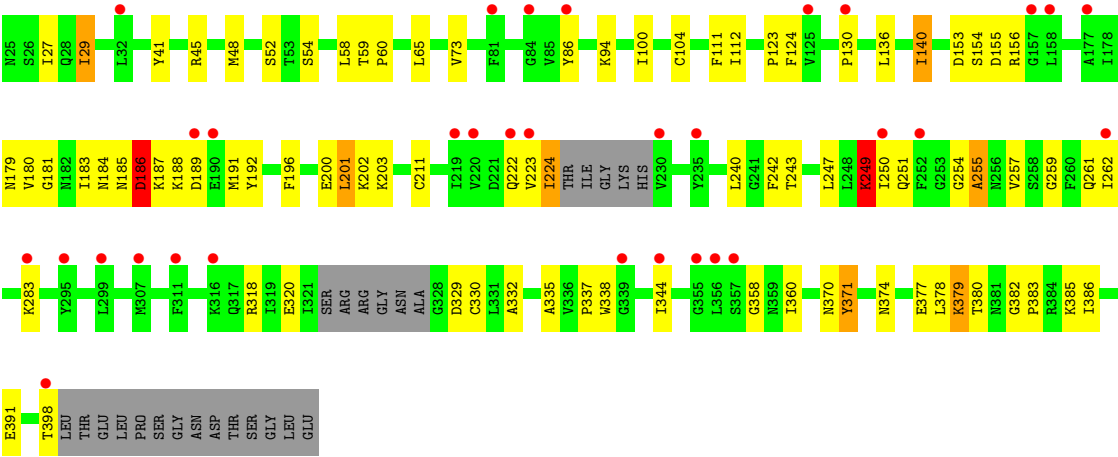


• Molecule 1: GLUTAMATE RECEPTOR 2



• Molecule 1: GLUTAMATE RECEPTOR 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	224.25Å 224.25Å 76.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 4.10 48.38 – 4.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.38-4.10) 99.9 (48.38-4.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.82 (at 4.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.290 , 0.354 0.313 , 0.358	Depositor DCC
R_{free} test set	802 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	152.3	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 285.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	8706	wwPDB-VP
Average B, all atoms (Å ²)	215.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.68	5/2961 (0.2%)	0.95	11/4003 (0.3%)
1	B	0.79	6/2961 (0.2%)	0.93	13/4003 (0.3%)
1	C	0.73	3/2961 (0.1%)	1.12	12/4003 (0.3%)
All	All	0.74	14/8883 (0.2%)	1.01	36/12009 (0.3%)

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	3
1	B	0	2
1	C	0	3
All	All	0	8

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	373	ILE	C-N	22.82	1.63	1.33
1	C	249	LYS	C-N	-19.67	1.06	1.33
1	A	249	LYS	C-N	-19.63	1.06	1.33
1	B	249	LYS	C-N	-19.62	1.06	1.33
1	C	371	TYR	C-N	17.68	1.58	1.33
1	C	130	PRO	C-N	17.52	1.57	1.33
1	B	371	TYR	C-N	-14.10	1.13	1.33
1	A	385	LYS	C-N	13.08	1.51	1.34
1	A	130	PRO	C-N	11.83	1.49	1.33
1	B	263	VAL	C-N	-9.54	1.17	1.33
1	A	261	GLN	C-N	7.89	1.43	1.34
1	B	130	PRO	C-N	-7.60	1.23	1.33
1	A	375	ILE	C-N	6.24	1.42	1.33
1	B	384	ARG	C-N	-6.17	1.24	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	130	PRO	O-C-N	27.65	157.30	123.01
1	C	130	PRO	CA-C-N	-24.26	86.72	121.42
1	C	130	PRO	C-N-CA	-24.26	86.72	121.42
1	A	130	PRO	O-C-N	17.31	144.47	123.01
1	A	130	PRO	CA-C-N	-16.45	97.90	121.42
1	A	130	PRO	C-N-CA	-16.45	97.90	121.42
1	B	261	GLN	CA-C-N	-13.86	99.45	121.35
1	B	261	GLN	C-N-CA	-13.86	99.45	121.35
1	C	261	GLN	CA-C-N	-13.85	99.46	121.35
1	C	261	GLN	C-N-CA	-13.85	99.46	121.35
1	C	261	GLN	O-C-N	12.37	140.29	123.34
1	B	261	GLN	O-C-N	12.35	140.25	123.34
1	A	186	ASP	OD1-CG-OD2	-12.23	93.55	122.90
1	C	186	ASP	OD1-CG-OD2	-12.20	93.62	122.90
1	B	186	ASP	OD1-CG-OD2	-12.20	93.62	122.90
1	B	186	ASP	CB-CG-OD2	-10.68	93.83	118.40
1	C	186	ASP	CB-CG-OD2	-10.64	93.92	118.40
1	A	186	ASP	CB-CG-OD2	-10.64	93.93	118.40
1	B	384	ARG	O-C-N	-10.24	111.58	123.25
1	C	371	TYR	CA-C-N	-9.99	107.77	122.65
1	C	371	TYR	C-N-CA	-9.99	107.77	122.65
1	A	249	LYS	O-C-N	-9.68	109.09	122.06
1	C	249	LYS	O-C-N	-9.67	109.11	122.06
1	B	249	LYS	O-C-N	-9.65	109.12	122.06
1	A	371	TYR	O-C-N	-9.12	112.62	123.10
1	B	384	ARG	CA-C-N	8.93	134.35	122.30
1	B	384	ARG	C-N-CA	8.93	134.35	122.30
1	A	261	GLN	CA-C-N	-8.87	109.00	121.77
1	A	261	GLN	C-N-CA	-8.87	109.00	121.77
1	B	130	PRO	CA-C-N	-8.66	108.57	120.87
1	B	130	PRO	C-N-CA	-8.66	108.57	120.87
1	B	130	PRO	O-C-N	8.28	133.27	123.01
1	A	261	GLN	O-C-N	8.13	134.48	123.34
1	C	379	LYS	CA-CB-CG	-6.85	100.39	114.10
1	A	379	LYS	CA-CB-CG	-6.85	100.40	114.10
1	B	379	LYS	CA-CB-CG	-6.85	100.40	114.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ASP	Sidechain
1	A	249	LYS	Peptide
1	A	371	TYR	Mainchain
1	B	186	ASP	Sidechain
1	B	249	LYS	Peptide
1	C	186	ASP	Sidechain
1	C	249	LYS	Peptide
1	C	371	TYR	Mainchain

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	2902	0	2852	138	1
1	B	2902	0	2852	94	8
1	C	2902	0	2852	85	9
All	All	8706	0	8556	305	11

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 18.

All (305) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LYS:O	1:A:250:ILE:HG12	1.22	1.34
1:B:249:LYS:O	1:B:250:ILE:HG13	1.16	1.28
1:C:249:LYS:O	1:C:250:ILE:HG13	1.16	1.25
1:A:224:ILE:HG13	1:C:224:ILE:CG1	1.69	1.22
1:A:224:ILE:CG1	1:C:224:ILE:HG13	1.69	1.21
1:A:208:ILE:HD13	1:A:236:ILE:HB	1.37	1.06
1:A:249:LYS:O	1:A:250:ILE:CG1	2.03	1.06
1:C:249:LYS:O	1:C:250:ILE:CG1	2.03	1.06
1:B:249:LYS:O	1:B:250:ILE:CG1	2.03	1.05
1:B:360:ILE:HD12	1:B:368:ARG:NH2	1.73	1.03
1:B:262:ILE:HG22	1:B:373:ILE:HD12	1.39	1.02
1:A:262:ILE:HD11	1:A:295:TYR:HB2	1.50	0.94
1:A:85:VAL:HG21	1:A:88:ILE:HD11	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:O	1:A:274:ILE:HD13	1.71	0.90
1:B:270:VAL:O	1:B:274:ILE:HD13	1.71	0.89
1:A:94:LYS:NZ	1:A:155:ASP:HA	1.88	0.88
1:A:94:LYS:CE	1:A:155:ASP:HA	2.06	0.86
1:A:314:LEU:CD1	1:A:344:ILE:HD13	2.06	0.85
1:A:208:ILE:CD1	1:A:236:ILE:HB	2.06	0.85
1:A:314:LEU:HD11	1:A:344:ILE:HD13	1.59	0.84
1:A:224:ILE:HG13	1:C:224:ILE:HG13	0.88	0.83
1:A:273:PHE:HD2	1:A:274:ILE:HD12	1.46	0.81
1:A:237:ILE:HD11	1:A:257:VAL:CG1	2.11	0.81
1:B:273:PHE:HD2	1:B:274:ILE:HD12	1.46	0.81
1:A:154:SER:HB3	1:A:179:ASN:HD21	1.46	0.80
1:B:154:SER:HB3	1:B:179:ASN:HD21	1.46	0.80
1:C:240:LEU:HD22	1:C:262:ILE:CG2	2.11	0.79
1:C:154:SER:HB3	1:C:179:ASN:HD21	1.46	0.79
1:A:254:GLY:O	1:A:255:ALA:CB	2.32	0.78
1:C:254:GLY:O	1:C:255:ALA:CB	2.32	0.77
1:B:254:GLY:O	1:B:255:ALA:CB	2.32	0.77
1:A:27:ILE:HG23	1:A:86:TYR:HD2	1.51	0.75
1:A:262:ILE:HD12	1:A:262:ILE:H	1.50	0.75
1:A:154:SER:HB3	1:A:179:ASN:ND2	2.02	0.74
1:B:27:ILE:HG23	1:B:86:TYR:HD2	1.52	0.74
1:B:375:ILE:HD13	1:B:395:MET:HE3	1.70	0.74
1:A:262:ILE:HD13	1:A:263:VAL:N	2.02	0.74
1:C:27:ILE:HG23	1:C:86:TYR:HD2	1.52	0.74
1:A:224:ILE:CG1	1:C:224:ILE:CG1	2.46	0.73
1:B:154:SER:HB3	1:B:179:ASN:ND2	2.02	0.73
1:C:154:SER:HB3	1:C:179:ASN:ND2	2.02	0.73
1:B:262:ILE:HG22	1:B:373:ILE:CD1	2.18	0.72
1:B:73:VAL:HG11	1:B:100:ILE:HD11	1.69	0.72
1:C:73:VAL:HG11	1:C:100:ILE:HD11	1.69	0.72
1:A:262:ILE:HD11	1:A:295:TYR:CB	2.19	0.71
1:A:321:ILE:HD13	1:A:321:ILE:H	1.55	0.71
1:A:237:ILE:HD11	1:A:257:VAL:HG13	1.73	0.71
1:B:112:ILE:HD13	1:B:126:ILE:HB	1.72	0.70
1:B:358:GLY:O	1:B:360:ILE:HD13	1.90	0.70
1:A:112:ILE:HD13	1:A:126:ILE:CB	2.23	0.69
1:A:94:LYS:HE3	1:A:154:SER:O	1.93	0.69
1:C:377:GLU:HG3	1:C:386:ILE:HD13	1.73	0.69
1:A:311:PHE:CE1	1:A:344:ILE:HD12	2.27	0.69
1:A:112:ILE:HD13	1:A:126:ILE:HB	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ILE:HD13	1:B:126:ILE:CB	2.22	0.68
1:A:174:GLN:NE2	1:B:174:GLN:NE2	2.40	0.68
1:C:240:LEU:HD22	1:C:262:ILE:HG23	1.74	0.67
1:A:176:THR:HG23	1:B:169:ALA:HB2	1.75	0.67
1:A:254:GLY:O	1:A:255:ALA:HB2	1.96	0.65
1:A:140:ILE:HD11	1:A:208:ILE:HD11	1.79	0.65
1:A:112:ILE:HD11	1:A:348:LEU:HD22	1.79	0.65
1:B:112:ILE:HD11	1:B:348:LEU:HD22	1.79	0.65
1:A:240:LEU:O	1:A:262:ILE:HD12	1.96	0.64
1:B:254:GLY:O	1:B:255:ALA:HB2	1.96	0.64
1:C:254:GLY:O	1:C:255:ALA:HB2	1.96	0.64
1:A:377:GLU:HG3	1:A:386:ILE:HD13	1.79	0.64
1:B:29:ILE:HD11	1:B:60:PRO:HB3	1.78	0.64
1:B:360:ILE:HD12	1:B:368:ARG:CZ	2.28	0.63
1:C:94:LYS:CE	1:C:155:ASP:HA	2.29	0.63
1:B:379:LYS:HG2	1:B:380:THR:N	2.14	0.63
1:A:85:VAL:HG21	1:A:88:ILE:CD1	2.28	0.62
1:A:94:LYS:HE3	1:A:155:ASP:HA	1.80	0.62
1:A:374:ASN:CG	1:A:385:LYS:HD2	2.25	0.62
1:C:180:VAL:HG12	1:C:180:VAL:O	2.00	0.62
1:B:180:VAL:HG12	1:B:180:VAL:O	2.00	0.61
1:A:237:ILE:N	1:A:237:ILE:HD12	2.14	0.61
1:C:379:LYS:HG2	1:C:380:THR:N	2.14	0.61
1:A:262:ILE:H	1:A:262:ILE:CD1	2.14	0.61
1:A:379:LYS:HG2	1:A:380:THR:N	2.14	0.61
1:B:262:ILE:CG2	1:B:373:ILE:HD12	2.24	0.61
1:A:180:VAL:HG12	1:A:180:VAL:O	2.00	0.61
1:B:249:LYS:O	1:B:249:LYS:HG2	2.01	0.61
1:C:370:ASN:N	1:C:391:GLU:OE2	2.22	0.60
1:B:257:VAL:HG23	1:B:378:LEU:HD22	1.83	0.60
1:C:224:ILE:C	1:C:224:ILE:HD13	2.27	0.60
1:C:257:VAL:HG23	1:C:378:LEU:HD22	1.83	0.60
1:A:94:LYS:CD	1:A:154:SER:O	2.50	0.60
1:A:224:ILE:C	1:A:224:ILE:HD13	2.27	0.60
1:A:48:MET:SD	1:A:60:PRO:HG3	2.42	0.59
1:A:249:LYS:O	1:A:249:LYS:HG2	2.01	0.59
1:A:251:GLN:NE2	1:A:382:GLY:HA2	2.17	0.59
1:A:257:VAL:HG23	1:A:378:LEU:HD22	1.83	0.59
1:B:48:MET:SD	1:B:60:PRO:HG3	2.42	0.59
1:C:48:MET:SD	1:C:60:PRO:HG3	2.42	0.59
1:A:377:GLU:CG	1:A:386:ILE:HG21	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:GLN:NE2	1:B:382:GLY:HA2	2.17	0.59
1:C:249:LYS:O	1:C:249:LYS:HG2	2.01	0.59
1:C:251:GLN:NE2	1:C:382:GLY:HA2	2.17	0.59
1:B:240:LEU:HD22	1:B:262:ILE:CG2	2.33	0.58
1:A:201:LEU:C	1:A:203:LYS:H	2.11	0.58
1:B:360:ILE:CD1	1:B:368:ARG:NH2	2.60	0.58
1:A:240:LEU:HD22	1:A:262:ILE:HG23	1.85	0.58
1:A:240:LEU:HD22	1:A:262:ILE:CG2	2.33	0.57
1:C:240:LEU:HB3	1:C:262:ILE:HG23	1.87	0.57
1:C:377:GLU:CG	1:C:386:ILE:HG21	2.35	0.57
1:C:94:LYS:HE3	1:C:155:ASP:HA	1.87	0.57
1:B:377:GLU:HG3	1:B:386:ILE:HD13	1.87	0.56
1:C:201:LEU:C	1:C:203:LYS:H	2.11	0.56
1:B:201:LEU:C	1:B:203:LYS:H	2.11	0.56
1:A:174:GLN:NE2	1:B:174:GLN:HE21	2.02	0.56
1:A:377:GLU:HG3	1:A:386:ILE:HG21	1.88	0.56
1:A:29:ILE:HD13	1:A:29:ILE:H	1.71	0.55
1:C:29:ILE:HD13	1:C:29:ILE:H	1.71	0.55
1:A:262:ILE:HD13	1:A:263:VAL:H	1.71	0.55
1:A:201:LEU:C	1:A:201:LEU:HD12	2.32	0.55
1:A:213:ARG:HH22	1:A:294:LYS:NZ	2.04	0.55
1:B:201:LEU:C	1:B:201:LEU:HD12	2.32	0.55
1:A:154:SER:H	1:A:181:GLY:HA3	1.72	0.55
1:C:136:LEU:O	1:C:140:ILE:HD13	2.07	0.55
1:A:126:ILE:N	1:A:126:ILE:HD12	2.23	0.54
1:B:375:ILE:HD13	1:B:395:MET:CE	2.37	0.54
1:C:154:SER:H	1:C:181:GLY:HA3	1.73	0.54
1:C:201:LEU:C	1:C:201:LEU:HD12	2.32	0.54
1:B:359:ASN:C	1:B:360:ILE:HD13	2.32	0.54
1:B:154:SER:H	1:B:181:GLY:HA3	1.73	0.54
1:A:243:THR:HG22	1:A:383:PRO:HG3	1.90	0.53
1:C:243:THR:HG22	1:C:383:PRO:HG3	1.91	0.53
1:A:145:TRP:CH2	1:A:236:ILE:HD13	2.44	0.53
1:B:243:THR:HG22	1:B:383:PRO:HG3	1.91	0.53
1:C:192:TYR:HB3	1:C:222:GLN:HG2	1.91	0.53
1:A:174:GLN:HE22	1:B:174:GLN:NE2	2.06	0.53
1:A:62:ILE:HD12	1:A:62:ILE:N	2.24	0.53
1:A:94:LYS:CE	1:A:154:SER:O	2.57	0.53
1:A:192:TYR:HB3	1:A:222:GLN:HG2	1.91	0.53
1:B:192:TYR:HB3	1:B:222:GLN:HG2	1.91	0.53
1:A:180:VAL:CG1	1:A:183:ILE:HD11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:GLU:HG3	1:C:386:ILE:HG21	1.90	0.52
1:B:187:LYS:H	1:B:187:LYS:HD2	1.74	0.52
1:A:174:GLN:HE22	1:B:174:GLN:HE21	1.57	0.52
1:B:377:GLU:HG3	1:B:386:ILE:HG21	1.92	0.52
1:C:187:LYS:H	1:C:187:LYS:HD2	1.74	0.52
1:A:187:LYS:H	1:A:187:LYS:HD2	1.74	0.51
1:B:154:SER:HB3	1:B:179:ASN:CG	2.35	0.51
1:A:154:SER:HB3	1:A:179:ASN:CG	2.35	0.51
1:A:262:ILE:CD1	1:A:262:ILE:N	2.72	0.51
1:A:262:ILE:HD13	1:A:263:VAL:HG23	1.91	0.51
1:A:377:GLU:CG	1:A:386:ILE:HD13	2.41	0.51
1:C:154:SER:HB3	1:C:179:ASN:CG	2.35	0.51
1:C:374:ASN:CG	1:C:385:LYS:HD2	2.35	0.51
1:C:112:ILE:N	1:C:112:ILE:HD12	2.26	0.51
1:C:257:VAL:CG2	1:C:378:LEU:HD22	2.41	0.51
1:A:257:VAL:CG2	1:A:378:LEU:HD22	2.41	0.51
1:C:196:PHE:O	1:C:200:GLU:HB2	2.11	0.51
1:B:196:PHE:O	1:B:200:GLU:HB2	2.12	0.50
1:A:314:LEU:CD1	1:A:344:ILE:CD1	2.86	0.50
1:A:196:PHE:O	1:A:200:GLU:HB2	2.11	0.50
1:C:377:GLU:CG	1:C:386:ILE:HD13	2.39	0.50
1:B:257:VAL:CG2	1:B:378:LEU:HD22	2.41	0.50
1:B:273:PHE:CD2	1:B:274:ILE:HD12	2.36	0.50
1:A:273:PHE:CD2	1:A:274:ILE:HD12	2.36	0.50
1:A:27:ILE:HD12	1:A:27:ILE:N	2.27	0.50
1:A:321:ILE:HD13	1:A:321:ILE:N	2.24	0.49
1:A:224:ILE:HD13	1:A:224:ILE:O	2.12	0.49
1:C:29:ILE:HD12	1:C:58:LEU:HB3	1.94	0.49
1:A:29:ILE:HD12	1:A:58:LEU:HB3	1.94	0.49
1:A:140:ILE:CD1	1:A:208:ILE:HD11	2.42	0.49
1:C:224:ILE:HD13	1:C:224:ILE:O	2.12	0.49
1:A:80:GLN:HB3	1:A:88:ILE:HD11	1.95	0.49
1:A:154:SER:OG	1:A:181:GLY:HA3	2.12	0.49
1:A:65:LEU:HD23	1:A:65:LEU:N	2.28	0.48
1:C:154:SER:OG	1:C:181:GLY:HA3	2.12	0.48
1:B:65:LEU:N	1:B:65:LEU:HD23	2.28	0.48
1:A:237:ILE:HD12	1:A:237:ILE:H	1.78	0.48
1:A:246:ASP:O	1:A:247:LEU:C	2.56	0.48
1:B:196:PHE:CE1	1:B:223:VAL:HG22	2.49	0.48
1:B:192:TYR:CE1	1:B:219:ILE:HD13	2.49	0.48
1:B:246:ASP:O	1:B:247:LEU:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:HD22	1:B:262:ILE:HG23	1.94	0.48
1:C:27:ILE:HG23	1:C:86:TYR:CD2	2.41	0.48
1:B:154:SER:OG	1:B:181:GLY:HA3	2.13	0.48
1:A:237:ILE:HD13	1:A:242:PHE:HE1	1.77	0.48
1:C:65:LEU:HD23	1:C:65:LEU:N	2.28	0.47
1:C:196:PHE:CE1	1:C:223:VAL:HG22	2.49	0.47
1:C:254:GLY:O	1:C:255:ALA:HB3	2.13	0.47
1:A:30:GLY:HA3	1:A:88:ILE:CD1	2.44	0.47
1:A:86:TYR:HD1	1:A:338:TRP:CH2	2.32	0.47
1:B:180:VAL:HG11	1:B:219:ILE:HD11	1.96	0.47
1:B:254:GLY:O	1:B:255:ALA:HB3	2.13	0.47
1:C:86:TYR:HD1	1:C:338:TRP:CH2	2.32	0.47
1:A:183:ILE:HD12	1:A:215:LYS:HD2	1.96	0.47
1:A:187:LYS:O	1:A:191:MET:HG3	2.15	0.47
1:B:86:TYR:HD1	1:B:338:TRP:CH2	2.33	0.47
1:A:184:ASN:C	1:A:186:ASP:N	2.73	0.47
1:B:41:TYR:CE2	1:B:45:ARG:HD2	2.50	0.47
1:B:240:LEU:HB3	1:B:262:ILE:HG23	1.97	0.47
1:C:188:LYS:HD3	1:C:189:ASP:N	2.31	0.47
1:A:377:GLU:OE2	1:A:386:ILE:HD13	2.14	0.46
1:C:187:LYS:O	1:C:191:MET:HG3	2.15	0.46
1:A:196:PHE:CE1	1:A:223:VAL:HG22	2.49	0.46
1:A:41:TYR:CE2	1:A:45:ARG:HD2	2.50	0.46
1:A:213:ARG:HH22	1:A:294:LYS:HZ2	1.62	0.46
1:B:73:VAL:HG11	1:B:100:ILE:CD1	2.43	0.46
1:B:188:LYS:HG2	1:B:192:TYR:CE2	2.51	0.46
1:A:188:LYS:HD3	1:A:189:ASP:N	2.30	0.46
1:B:188:LYS:HD3	1:B:189:ASP:N	2.30	0.46
1:B:377:GLU:CG	1:B:386:ILE:HG21	2.46	0.46
1:C:188:LYS:HG2	1:C:192:TYR:CE2	2.51	0.46
1:B:375:ILE:CD1	1:B:395:MET:HE3	2.44	0.46
1:A:188:LYS:HG2	1:A:192:TYR:CE2	2.51	0.46
1:C:41:TYR:CE2	1:C:45:ARG:HD2	2.50	0.46
1:B:184:ASN:C	1:B:186:ASP:N	2.73	0.45
1:B:209:LEU:HD12	1:B:237:ILE:CD1	2.45	0.45
1:B:187:LYS:O	1:B:191:MET:HG3	2.15	0.45
1:B:29:ILE:C	1:B:29:ILE:HD12	2.42	0.45
1:C:73:VAL:HG11	1:C:100:ILE:CD1	2.43	0.45
1:C:201:LEU:C	1:C:203:LYS:N	2.75	0.45
1:B:187:LYS:HD2	1:B:187:LYS:N	2.32	0.45
1:C:187:LYS:HD2	1:C:187:LYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:C	1:A:203:LYS:N	2.75	0.45
1:C:184:ASN:C	1:C:186:ASP:N	2.73	0.45
1:A:140:ILE:HD11	1:A:208:ILE:CD1	2.46	0.45
1:A:29:ILE:HD13	1:A:59:THR:C	2.42	0.45
1:C:29:ILE:HD13	1:C:59:THR:C	2.42	0.45
1:A:187:LYS:HD2	1:A:187:LYS:N	2.32	0.44
1:C:186:ASP:C	1:C:188:LYS:H	2.25	0.44
1:A:180:VAL:HG12	1:A:183:ILE:HD11	1.98	0.44
1:C:183:ILE:C	1:C:185:ASN:H	2.25	0.44
1:C:335:ALA:O	1:C:337:PRO:HD3	2.18	0.44
1:B:183:ILE:C	1:B:185:ASN:H	2.25	0.44
1:A:176:THR:HG23	1:B:169:ALA:CB	2.43	0.44
1:A:237:ILE:CD1	1:A:257:VAL:CG1	2.90	0.44
1:A:335:ALA:O	1:A:337:PRO:HD3	2.18	0.44
1:B:100:ILE:N	1:B:100:ILE:HD12	2.33	0.44
1:A:379:LYS:CG	1:A:380:THR:N	2.81	0.44
1:C:379:LYS:CG	1:C:380:THR:N	2.81	0.44
1:A:236:ILE:CD1	1:A:236:ILE:N	2.81	0.44
1:B:335:ALA:O	1:B:337:PRO:HD3	2.17	0.43
1:A:48:MET:O	1:A:52:SER:HB3	2.18	0.43
1:A:311:PHE:CE1	1:A:344:ILE:CD1	2.98	0.43
1:B:48:MET:O	1:B:52:SER:HB3	2.18	0.43
1:B:153:ASP:HB3	1:B:156:ARG:HB2	2.00	0.43
1:B:360:ILE:HD13	1:B:360:ILE:N	2.33	0.43
1:C:153:ASP:HB3	1:C:156:ARG:HB2	2.00	0.43
1:B:123:PRO:O	1:B:124:PHE:HB2	2.18	0.43
1:A:224:ILE:CG1	1:C:224:ILE:HG12	2.45	0.43
1:A:254:GLY:O	1:A:255:ALA:HB3	2.13	0.43
1:C:48:MET:O	1:C:52:SER:HB3	2.18	0.43
1:C:100:ILE:HD12	1:C:100:ILE:N	2.33	0.43
1:B:249:LYS:O	1:B:250:ILE:CB	2.55	0.43
1:A:183:ILE:C	1:A:185:ASN:H	2.26	0.43
1:A:94:LYS:HZ1	1:A:155:ASP:HA	1.76	0.43
1:A:377:GLU:HG3	1:A:386:ILE:CG2	2.48	0.43
1:A:377:GLU:CD	1:A:386:ILE:HG21	2.43	0.43
1:A:153:ASP:HB3	1:A:156:ARG:HB2	2.00	0.43
1:B:27:ILE:HG23	1:B:86:TYR:CD2	2.41	0.43
1:C:123:PRO:O	1:C:124:PHE:HB2	2.18	0.43
1:A:186:ASP:C	1:A:188:LYS:H	2.25	0.43
1:B:379:LYS:CG	1:B:380:THR:N	2.81	0.43
1:A:123:PRO:O	1:A:124:PHE:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:CYS:SG	1:B:111:PHE:HB2	2.59	0.42
1:B:154:SER:HB3	1:B:179:ASN:OD1	2.19	0.42
1:B:186:ASP:C	1:B:188:LYS:H	2.25	0.42
1:A:235:TYR:O	1:A:236:ILE:HD12	2.19	0.42
1:B:338:TRP:CH2	1:B:344:ILE:HD12	2.54	0.42
1:C:140:ILE:N	1:C:140:ILE:CD1	2.82	0.42
1:C:242:PHE:CD1	1:C:259:GLY:HA3	2.54	0.42
1:A:104:CYS:SG	1:A:111:PHE:HB2	2.59	0.42
1:A:329:ASP:HB3	1:A:332:ALA:HB2	2.02	0.42
1:A:29:ILE:HD13	1:A:29:ILE:N	2.34	0.42
1:C:154:SER:HB3	1:C:179:ASN:OD1	2.19	0.42
1:B:65:LEU:HD23	1:B:65:LEU:H	1.85	0.42
1:C:104:CYS:SG	1:C:111:PHE:HB2	2.59	0.42
1:A:270:VAL:O	1:A:274:ILE:CD1	2.56	0.42
1:B:215:LYS:HE2	1:B:215:LYS:HB2	1.86	0.42
1:B:329:ASP:HB3	1:B:332:ALA:HB2	2.02	0.42
1:C:29:ILE:HD13	1:C:29:ILE:N	2.34	0.42
1:A:154:SER:HB3	1:A:179:ASN:OD1	2.19	0.42
1:B:242:PHE:CD1	1:B:259:GLY:HA3	2.54	0.42
1:A:235:TYR:C	1:A:236:ILE:HD12	2.45	0.42
1:A:62:ILE:HD12	1:A:62:ILE:H	1.84	0.42
1:B:180:VAL:O	1:B:180:VAL:CG1	2.68	0.42
1:A:27:ILE:HG23	1:A:86:TYR:CD2	2.41	0.41
1:A:71:PHE:HD1	1:B:103:PHE:CD2	2.38	0.41
1:B:112:ILE:HD13	1:B:126:ILE:HG13	2.02	0.41
1:C:398:THR:O	1:C:398:THR:HG22	2.19	0.41
1:A:113:THR:HA	1:A:114:PRO:HD3	1.88	0.41
1:A:153:ASP:HB2	1:A:211:CYS:HA	2.03	0.41
1:A:202:LYS:HG2	1:A:202:LYS:O	2.20	0.41
1:C:338:TRP:CH2	1:C:344:ILE:HD12	2.55	0.41
1:A:237:ILE:CD1	1:A:257:VAL:HG12	2.50	0.41
1:C:153:ASP:HB2	1:C:211:CYS:HA	2.03	0.41
1:C:65:LEU:HD23	1:C:65:LEU:H	1.84	0.41
1:C:180:VAL:O	1:C:180:VAL:CG1	2.68	0.41
1:C:202:LYS:HG2	1:C:202:LYS:O	2.20	0.41
1:C:329:ASP:HB3	1:C:332:ALA:HB2	2.02	0.41
1:A:30:GLY:HA3	1:A:88:ILE:HD13	2.02	0.41
1:A:112:ILE:HD13	1:A:126:ILE:CG1	2.51	0.41
1:C:100:ILE:HD12	1:C:100:ILE:H	1.86	0.41
1:B:153:ASP:HB2	1:B:211:CYS:HA	2.03	0.41
1:B:202:LYS:HG2	1:B:202:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ASP:C	1:C:188:LYS:N	2.79	0.40
1:C:242:PHE:O	1:C:247:LEU:HD23	2.21	0.40
1:C:358:GLY:O	1:C:360:ILE:HD12	2.21	0.40
1:C:377:GLU:HB2	1:C:386:ILE:CG2	2.51	0.40
1:B:112:ILE:HD13	1:B:126:ILE:CG1	2.51	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:SER:CB	1:C:318:ARG:NH2[8_554]	1.28	0.92
1:B:245:GLY:CA	1:C:283:LYS:NZ[3_444]	1.37	0.83
1:B:245:GLY:C	1:C:283:LYS:NZ[3_444]	1.48	0.72
1:C:54:SER:OG	1:C:318:ARG:NH2[8_554]	1.73	0.47
1:B:245:GLY:O	1:C:283:LYS:CE[3_444]	1.74	0.46
1:B:245:GLY:C	1:C:283:LYS:CE[3_444]	1.84	0.36
1:B:59:THR:CG2	1:B:334:PRO:CG[3_444]	1.87	0.33
1:B:252:PHE:CZ	1:C:48:MET:CE[3_444]	2.00	0.20
1:B:252:PHE:CE2	1:C:48:MET:CE[3_444]	2.05	0.15
1:B:246:ASP:N	1:C:283:LYS:NZ[3_444]	2.08	0.12
1:A:60:PRO:O	1:A:333:ASN:O[4_545]	2.13	0.07

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	357/388 (92%)	336 (94%)	20 (6%)	1 (0%)	36	70
1	B	357/388 (92%)	336 (94%)	20 (6%)	1 (0%)	36	70
1	C	357/388 (92%)	335 (94%)	21 (6%)	1 (0%)	36	70
All	All	1071/1164 (92%)	1007 (94%)	61 (6%)	3 (0%)	36	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ALA
1	B	255	ALA
1	C	255	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/336 (94%)	307 (97%)	9 (3%)	38	59
1	B	316/336 (94%)	311 (98%)	5 (2%)	55	69
1	C	316/336 (94%)	310 (98%)	6 (2%)	50	67
All	All	948/1008 (94%)	928 (98%)	20 (2%)	47	65

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	112	ILE
1	A	201	LEU
1	A	224	ILE
1	A	236	ILE
1	A	262	ILE
1	A	320	GLU
1	A	321	ILE
1	A	330	CYS
1	B	112	ILE
1	B	201	LEU
1	B	320	GLU
1	B	330	CYS
1	B	360	ILE
1	C	29	ILE
1	C	140	ILE
1	C	201	LEU
1	C	224	ILE

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Mol	Chain	Res	Type
1	C	320	GLU
1	C	330	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	182	ASN
1	B	174	GLN
1	B	182	ASN
1	C	174	GLN
1	C	182	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	4
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	373:ILE	C	374:ASN	N	1.63
1	B	263:VAL	C	264:ASP	N	1.17
1	B	371:TYR	C	372:THR	N	1.13
1	B	249:LYS	C	250:ILE	N	1.07
1	A	249:LYS	C	250:ILE	N	1.06
1	C	249:LYS	C	250:ILE	N	1.06

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	363/388 (93%)	0.71	36 (9%)	13 15	88, 195, 325, 398	0
1	B	363/388 (93%)	0.74	43 (11%)	9 12	111, 194, 317, 465	0
1	C	363/388 (93%)	0.64	32 (8%)	15 18	132, 230, 315, 427	0
All	All	1089/1164 (93%)	0.69	111 (10%)	12 15	88, 208, 320, 465	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	357	SER	9.0
1	B	245	GLY	5.9
1	B	235	TYR	5.7
1	C	222	GLN	5.1
1	B	153	ASP	5.1
1	B	155	ASP	4.8
1	A	155	ASP	4.4
1	A	219	ILE	4.4
1	C	235	TYR	4.4
1	A	250	ILE	4.3
1	C	311	PHE	4.2
1	C	262	ILE	4.2
1	B	107	LEU	4.1
1	B	230	VAL	3.9
1	B	219	ILE	3.9
1	A	222	GLN	3.8
1	A	338	TRP	3.8
1	A	336	VAL	3.8
1	A	311	PHE	3.6
1	A	182	ASN	3.5
1	A	230	VAL	3.5
1	A	321	ILE	3.5
1	C	219	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	254	GLY	3.4
1	C	190	GLU	3.3
1	C	81	PHE	3.3
1	C	299	LEU	3.3
1	B	246	ASP	3.2
1	C	356	LEU	3.2
1	B	277	TRP	3.2
1	B	86	TYR	3.1
1	C	344	ILE	3.1
1	A	223	VAL	3.1
1	B	212	GLU	3.0
1	A	86	TYR	3.0
1	C	223	VAL	3.0
1	B	336	VAL	3.0
1	A	220	VAL	2.9
1	A	252	PHE	2.8
1	A	154	SER	2.8
1	B	335	ALA	2.8
1	A	224	ILE	2.7
1	B	370	ASN	2.7
1	C	86	TYR	2.7
1	B	369	ILE	2.7
1	B	330	CYS	2.7
1	A	328	GLY	2.6
1	A	125	VAL	2.6
1	B	249	LYS	2.6
1	B	255	ALA	2.6
1	A	157	GLY	2.5
1	B	248	LEU	2.5
1	B	383	PRO	2.5
1	B	116	PHE	2.5
1	A	190	GLU	2.5
1	B	222	GLN	2.5
1	B	224	ILE	2.5
1	B	190	GLU	2.5
1	C	220	VAL	2.5
1	C	250	ILE	2.4
1	B	334	PRO	2.4
1	B	280	LEU	2.4
1	A	357	SER	2.4
1	A	109	VAL	2.3
1	C	316	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	84	GLY	2.3
1	B	253	GLY	2.3
1	C	125	VAL	2.3
1	C	252	PHE	2.3
1	A	337	PRO	2.3
1	C	295	TYR	2.3
1	B	288	ALA	2.3
1	A	150	TYR	2.2
1	A	245	GLY	2.2
1	A	255	ALA	2.2
1	B	276	ARG	2.2
1	C	157	GLY	2.2
1	C	339	GLY	2.2
1	A	249	LYS	2.2
1	C	189	ASP	2.2
1	C	355	GLY	2.2
1	B	59	THR	2.2
1	C	32	LEU	2.2
1	A	243	THR	2.2
1	A	295	TYR	2.2
1	A	239	ASN	2.2
1	B	111	PHE	2.1
1	A	58	LEU	2.1
1	A	118	THR	2.1
1	A	263	VAL	2.1
1	C	230	VAL	2.1
1	B	81	PHE	2.1
1	B	250	ILE	2.1
1	C	283	LYS	2.1
1	C	158	LEU	2.1
1	B	278	SER	2.1
1	B	343	GLU	2.1
1	B	125	VAL	2.1
1	C	307	MET	2.1
1	B	289	HIS	2.1
1	C	130	PRO	2.1
1	B	328	GLY	2.1
1	A	340	GLN	2.1
1	B	251	GLN	2.1
1	B	337	PRO	2.1
1	A	50	GLN	2.0
1	C	398	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	344	ILE	2.0
1	B	359	ASN	2.0
1	C	177	ALA	2.0
1	B	122	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.