Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:16 AM GMT

PDB ID	:	2WJX
Title	:	CRYSTAL STRUCTURE OF THE HUMAN IONOTROPIC GLUTAMATE RECEPTOR GLUR2 ATD REGION AT 4.1 A 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
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:

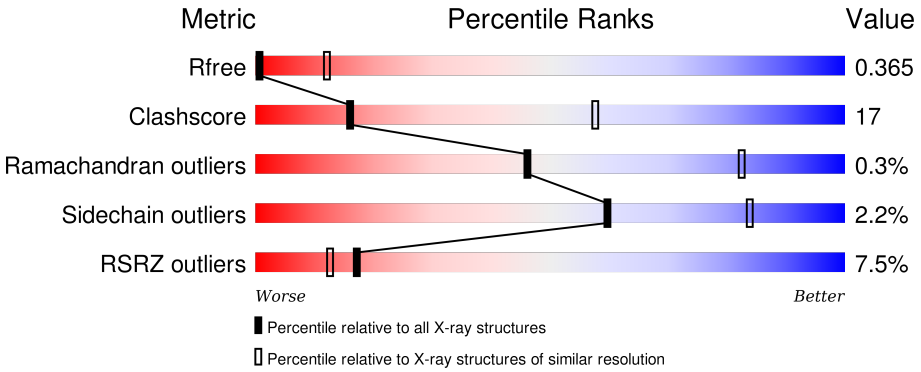
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.10 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}	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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	388	6% 67% 23% • • 6%
1	B	388	7% 70% 22% • 6%
1	C	388	8% 72% 19% • • 6%

2 Entry composition (i)

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.

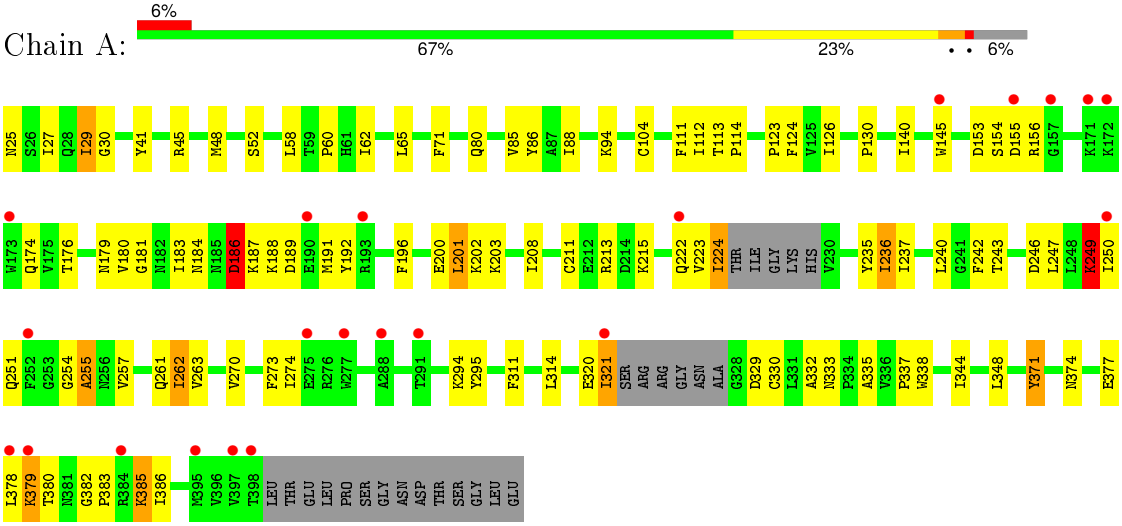
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2902	1852	489	551	10			
1	B	363	Total	C	N	O	S	0	0	0
			2902	1852	489	551	10			
1	C	363	Total	C	N	O	S	0	0	0
			2902	1852	489	551	10			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

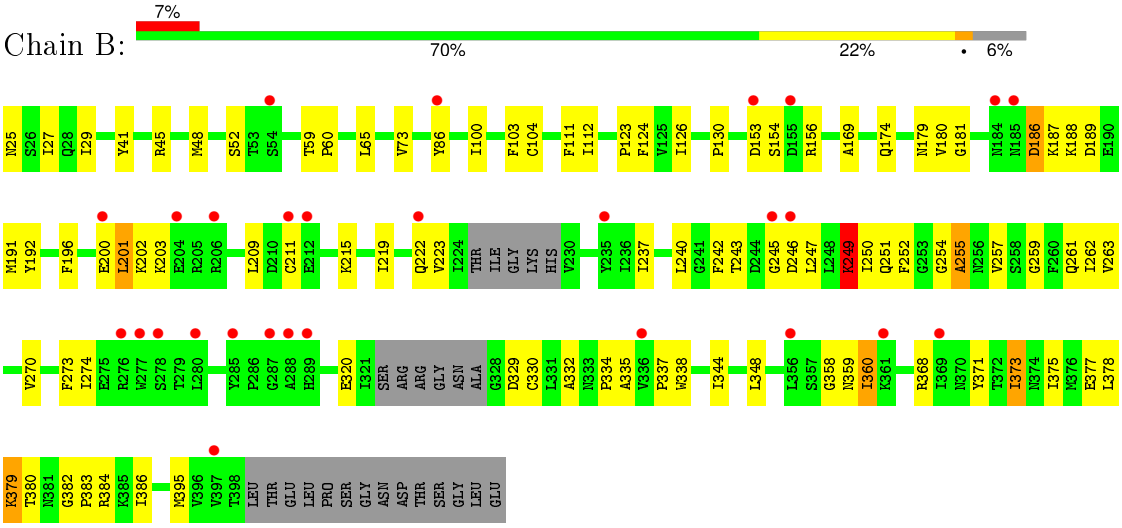
- Molecule 1: GLUTAMATE RECEPTOR 2

Chain A:



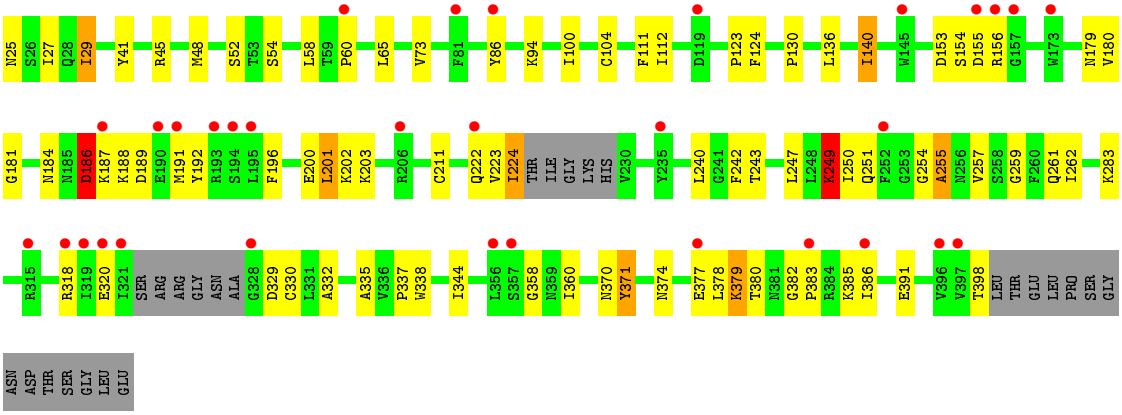
- Molecule 1: GLUTAMATE RECEPTOR 2

Chain B:



- Molecule 1: GLUTAMATE RECEPTOR 2

Chain C:


N25 S26 I27 Q28 I29 Y41 R45 M48 S52 T53 S54 L58 T59 P60 L65 V73 F81 Y86 K94 I100 C104 F111 I112 D119 P123 F124 P130 L136 I140 W145 D153 S154 D155 R156 G157 W173 N179 V180
G181 N184 N185 D186 K187 K188 D189 E190 M191 Y192 R193 S194 L195 F196 E200 L201 K202 K203 R206 C211 Q222 V223 I224 THR ILE GLY LYS HIS V230 Y235 L240 G241 F242 T243 L247 L248 K249 I250 Q251 F252 G253 G254 A255 N256 V257 S258 G259 P260 Q261 I262 K283
R315 R318 I319 E320 I321 SER ARG ARG GLY ASN ALA G328 D329 C330 L331 A332 A335 V336 P337 W338 I344 L356 S357 G358 N359 I360 N370 Y371 N374 E377 L378 K379 T380 N381 G382 P383 R384 K385 I386 E391 V396 V397 T398 LEU THR GLU LEU PRO SER GLY
ASN ASP THR SER GLY LEU GLU

4 Data and refinement statistics (i)

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) 100.0 (48.38-4.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.82 (at 4.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.290 , 0.354 0.307 , 0.365	Depositor DCC
R_{free} test set	801 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	152.3	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 196.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 15948 reflections	Xtriage
F_o,F_c correlation	0.82	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.*

[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	0.47	3/2961 (0.1%)	0.82	12/4003 (0.3%)
1	B	0.54	4/2961 (0.1%)	0.81	12/4003 (0.3%)
1	C	0.50	3/2961 (0.1%)	0.92	13/4003 (0.3%)
All	All	0.51	10/8883 (0.1%)	0.85	37/12009 (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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	373	ILE	C-N	12.84	1.63	1.34
1	C	249	LYS	C-N	-11.81	1.06	1.34
1	A	249	LYS	C-N	-11.79	1.06	1.34
1	B	249	LYS	C-N	-11.78	1.06	1.34
1	C	371	TYR	C-N	10.70	1.58	1.34
1	C	130	PRO	C-N	10.26	1.57	1.34
1	B	371	TYR	C-N	-9.08	1.13	1.34
1	A	385	LYS	C-N	7.43	1.51	1.34
1	B	263	VAL	C-N	-7.06	1.17	1.34
1	A	130	PRO	C-N	6.84	1.49	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	186	ASP	CB-CG-OD2	-27.18	93.83	118.30
1	C	186	ASP	CB-CG-OD2	-27.09	93.92	118.30
1	A	186	ASP	CB-CG-OD2	-27.08	93.93	118.30
1	C	130	PRO	O-C-N	21.62	157.30	122.70
1	C	130	PRO	CA-C-N	-16.23	81.49	117.20
1	A	186	ASP	OD1-CG-OD2	-15.66	93.55	123.30
1	C	186	ASP	OD1-CG-OD2	-15.62	93.62	123.30
1	B	186	ASP	OD1-CG-OD2	-15.62	93.62	123.30
1	C	130	PRO	C-N-CA	-13.99	86.72	121.70
1	A	130	PRO	O-C-N	13.61	144.47	122.70
1	C	261	GLN	O-C-N	10.99	140.29	122.70
1	B	261	GLN	O-C-N	10.97	140.25	122.70
1	A	130	PRO	CA-C-N	-10.22	94.72	117.20
1	A	130	PRO	C-N-CA	-9.52	97.90	121.70
1	C	261	GLN	CA-C-N	-9.04	97.32	117.20
1	B	261	GLN	CA-C-N	-9.03	97.34	117.20
1	B	261	GLN	C-N-CA	-8.90	99.45	121.70
1	C	261	GLN	C-N-CA	-8.90	99.46	121.70
1	A	249	LYS	O-C-N	-8.51	109.09	122.70
1	C	249	LYS	O-C-N	-8.50	109.11	122.70
1	B	249	LYS	O-C-N	-8.48	109.12	122.70
1	A	261	GLN	O-C-N	7.36	134.48	122.70
1	B	384	ARG	O-C-N	-6.95	111.58	122.70
1	B	130	PRO	O-C-N	6.61	133.27	122.70
1	A	371	TYR	O-C-N	-6.30	112.62	122.70
1	C	379	LYS	CA-CB-CG	-5.91	100.39	113.40
1	A	379	LYS	CA-CB-CG	-5.91	100.40	113.40
1	B	379	LYS	CA-CB-CG	-5.91	100.40	113.40
1	A	249	LYS	CA-C-N	5.78	129.92	117.20
1	C	249	LYS	CA-C-N	5.78	129.91	117.20
1	B	249	LYS	CA-C-N	5.76	129.88	117.20
1	A	261	GLN	CA-C-N	-5.60	104.89	117.20
1	C	371	TYR	C-N-CA	-5.57	107.77	121.70
1	C	371	TYR	CA-C-N	-5.56	104.97	117.20
1	B	130	PRO	C-N-CA	-5.25	108.57	121.70
1	A	261	GLN	C-N-CA	-5.08	109.00	121.70
1	B	384	ARG	C-N-CA	5.06	134.35	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ASP	Sidechain

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Mol	Chain	Res	Type	Group
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 (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	2902	0	2852	134	1
1	B	2902	0	2849	89	8
1	C	2902	0	2852	81	9
All	All	8706	0	8553	292	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 17.

All (292) 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:B:273:PHE:HD2	1:B:274:ILE:HD12	1.46	0.81
1:A:237:ILE:HD11	1:A:257:VAL:CG1	2.11	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:H	1:A:262:ILE:HD12	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: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:H	1:A:321:ILE:HD13	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
1:B:112:ILE:HD13	1:B:126:ILE:CB	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:254:GLY:O	1:C:255:ALA:HB2	1.96	0.64
1:B:254:GLY:O	1:B: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:A:379:LYS:HG2	1:A:380:THR:N	2.14	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:C:180:VAL:O	1:C:180:VAL:HG12	2.00	0.62
1:B:180:VAL:O	1:B:180:VAL:HG12	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:B:262:ILE:CG2	1:B:373:ILE:HD12	2.24	0.61
1:B:249:LYS:HG2	1:B:249:LYS:O	2.01	0.61
1:A:180:VAL:HG12	1:A:180:VAL:O	2.00	0.61
1:C:370:ASN:N	1:C:391:GLU:OE2	2.22	0.60
1:C:257:VAL:HG23	1:C:378:LEU:HD22	1.83	0.60
1:B:257:VAL:HG23	1:B:378:LEU:HD22	1.83	0.60
1:A:94:LYS:CD	1:A:154:SER:O	2.50	0.60
1:A:48:MET:SD	1:A:60:PRO:HG3	2.42	0.59
1:A:249:LYS:HG2	1:A:249:LYS:O	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
1:C:249:LYS:O	1:C:249:LYS:HG2	2.01	0.59
1:B:251:GLN:NE2	1:B:382:GLY:HA2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:374:ASN:CG	1:A:385:LYS:HD2	2.25	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: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:C:224:ILE:C	1:C:224:ILE:HD13	2.27	0.55
1:A:224:ILE:HD13	1:A:224:ILE:C	2.27	0.55
1:A:29:ILE:HD13	1:A:29:ILE:H	1.71	0.55
1:C:29:ILE:H	1:C:29:ILE:HD13	1.71	0.55
1:A:262:ILE:HD13	1:A:263:VAL:H	1.71	0.55
1:A:213:ARG:HH22	1:A:294:LYS:NZ	2.04	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:HD12	1:A:126:ILE:N	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:B:154:SER:H	1:B:181:GLY:HA3	1.73	0.54
1:A:201:LEU:C	1:A:203:LYS:H	2.11	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:B:192:TYR:HB3	1:B:222:GLN:HG2	1.91	0.53
1:A:192:TYR:HB3	1:A:222:GLN:HG2	1.91	0.53
1:A:180:VAL:CG1	1:A:183:ILE:HD11	2.39	0.52
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:C:201:LEU:C	1:C:203:LYS:H	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:C	1:B:203:LYS:H	2.11	0.51
1:A:262:ILE:N	1:A:262:ILE:CD1	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:257:VAL:CG2	1:C:378:LEU:HD22	2.41	0.51
1:C:112:ILE:HD12	1:C:112:ILE:N	2.26	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:C:377:GLU:CG	1:C:386:ILE:HD13	2.39	0.50
1:A:201:LEU:HD12	1:A:201:LEU:C	2.32	0.50
1:A:196:PHE:O	1:A:200:GLU:HB2	2.11	0.50
1:B:273:PHE:CD2	1:B:274:ILE:HD12	2.36	0.50
1:B:257:VAL:CG2	1:B:378:LEU:HD22	2.41	0.50
1:B:201:LEU:C	1:B:201:LEU:HD12	2.32	0.50
1:A:273:PHE:CD2	1:A:274:ILE:HD12	2.36	0.50
1:A:27:ILE:N	1:A:27:ILE:HD12	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:C:201:LEU:HD12	1:C:201:LEU:C	2.32	0.49
1:C:224:ILE:O	1:C:224:ILE:HD13	2.12	0.49
1:A:140:ILE:CD1	1:A:208:ILE:HD11	2.42	0.49
1:B:359:ASN:C	1:B:360:ILE:HD13	2.32	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:94:LYS:HZ2	1:A:155:ASP:HA	1.76	0.49
1:C:154:SER:OG	1:C:181:GLY:HA3	2.12	0.48
1:A:65:LEU:HD23	1:A:65:LEU:N	2.28	0.48
1:B:65:LEU:HD23	1:B:65:LEU:N	2.28	0.48
1:A:237:ILE:H	1:A:237:ILE:HD12	1.78	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: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:254:GLY:O	1:C:255:ALA:HB3	2.13	0.47
1:C:196:PHE:CE1	1:C:223:VAL:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:LEU:HD23	1:C:65:LEU:N	2.28	0.47
1:A:30:GLY:HA3	1:A:88:ILE:CD1	2.44	0.47
1:B:254:GLY:O	1:B:255:ALA:HB3	2.13	0.47
1:A:86:TYR:HD1	1:A:338:TRP:CH2	2.32	0.47
1:C:86:TYR:HD1	1:C:338:TRP:CH2	2.32	0.47
1:B:180:VAL:HG11	1:B:219:ILE:HD11	1.96	0.47
1:B:86:TYR:HD1	1:B:338:TRP:CH2	2.33	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:154:SER:HB3	1:B:179:ASN:CG	2.35	0.47
1:A:154:SER:HB3	1:A:179:ASN:CG	2.35	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:C:154:SER:HB3	1:C:179:ASN:CG	2.35	0.46
1:A:196:PHE:CE1	1:A:223:VAL:HG22	2.49	0.46
1:C:374:ASN:CG	1:C:385:LYS:HD2	2.35	0.46
1:A:41:TYR:CE2	1:A:45:ARG:HD2	2.50	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: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:A:188:LYS:HD3	1:A:189:ASP:N	2.30	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: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:C:73:VAL:HG11	1:C:100:ILE:CD1	2.43	0.45
1:B:187:LYS:N	1:B:187:LYS:HD2	2.32	0.45
1:C:187:LYS:N	1:C:187:LYS:HD2	2.32	0.45
1:A:140:ILE:HD11	1:A:208:ILE:CD1	2.46	0.45
1:A:187:LYS:N	1:A:187:LYS:HD2	2.32	0.44
1:A:180:VAL:HG12	1:A:183:ILE:HD11	1.98	0.44
1:C:335:ALA:O	1:C:337:PRO:HD3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:236:ILE:CD1	2.81	0.44
1:B:335:ALA:O	1:B:337:PRO:HD3	2.17	0.43
1:A:311:PHE:CE1	1:A:344:ILE:CD1	2.98	0.43
1:A:48:MET:O	1:A:52:SER:HB3	2.18	0.43
1:A:246:ASP:O	1:A:247:LEU:C	2.56	0.43
1:B:360:ILE:N	1:B:360:ILE:HD13	2.33	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: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:B:246:ASP:O	1:B:247:LEU:C	2.56	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:100:ILE:HD12	1:C:100:ILE:N	2.33	0.43
1:C:48:MET:O	1:C:52:SER:HB3	2.18	0.43
1:B:249:LYS:O	1:B:250:ILE:CB	2.55	0.43
1:A:377:GLU:HG3	1:A:386:ILE:CG2	2.48	0.43
1:B:27:ILE:HG23	1:B:86:TYR:CD2	2.41	0.43
1:A:153:ASP:HB3	1:A:156:ARG:HB2	2.00	0.43
1:C:123:PRO:O	1:C:124:PHE:HB2	2.18	0.43
1:B:379:LYS:CG	1:B:380:THR:N	2.81	0.43
1:B:154:SER:HB3	1:B:179:ASN:OD1	2.19	0.42
1:B:104:CYS:SG	1:B:111:PHE:HB2	2.59	0.42
1:A:123:PRO:O	1:A:124:PHE:HB2	2.18	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:CD1	1:C:140:ILE:N	2.82	0.42
1:C:242:PHE:CD1	1:C:259:GLY:HA3	2.54	0.42
1:A:213:ARG:HH22	1:A:294:LYS:HZ2	1.65	0.42
1:A:329:ASP:HB3	1:A:332:ALA:HB2	2.02	0.42
1:A:104:CYS:SG	1:A:111:PHE:HB2	2.59	0.42
1:C:154:SER:HB3	1:C:179:ASN:OD1	2.19	0.42
1:A:29:ILE:HD13	1:A:29:ILE:N	2.34	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:C:29:ILE:N	1:C:29:ILE:HD13	2.34	0.42
1:B:329:ASP:HB3	1:B:332:ALA:HB2	2.02	0.42
1:C:184:ASN:C	1:C:186:ASP:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LYS:HB2	1:B:215:LYS:HE2	1.86	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:62:ILE:HD12	1:A:62:ILE:H	1.84	0.42
1:A:94:LYS:HZ1	1:A:155:ASP:HA	1.77	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: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:71:PHE:HD1	1:B:103:PHE:CD2	2.38	0.41
1:A:184:ASN:C	1:A:186:ASP:N	2.73	0.41
1:C:338:TRP:CH2	1:C:344:ILE:HD12	2.55	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:A:113:THR:HA	1:A:114:PRO:HD3	1.88	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:H	1:C:65:LEU:HD23	1.84	0.41
1:C:180:VAL:O	1:C:180:VAL:CG1	2.68	0.41
1:C:202:LYS:O	1:C:202:LYS:HG2	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:C:100:ILE:HD12	1:C:100:ILE:H	1.86	0.41
1:A:112:ILE:HD13	1:A:126:ILE:CG1	2.51	0.41
1:B:153:ASP:HB2	1:B:211:CYS:HA	2.03	0.41
1:B:202:LYS:O	1:B:202:LYS:HG2	2.20	0.41
1:B:29:ILE:C	1:B:29:ILE:HD12	2.42	0.40
1:C:201:LEU:C	1:C:203:LYS:N	2.75	0.40
1:C:377:GLU:HB2	1:C:386:ILE:CG2	2.51	0.40
1:A:201:LEU:C	1:A:203:LYS:N	2.75	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	46 82
1	B	357/388 (92%)	336 (94%)	20 (6%)	1 (0%)	46 82
1	C	357/388 (92%)	335 (94%)	21 (6%)	1 (0%)	46 82
All	All	1071/1164 (92%)	1007 (94%)	61 (6%)	3 (0%)	46 82

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 (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	316/336 (94%)	307 (97%)	9 (3%)	51	80
1	B	316/336 (94%)	311 (98%)	5 (2%)	70	88
1	C	316/336 (94%)	309 (98%)	7 (2%)	60	84
All	All	948/1008 (94%)	927 (98%)	21 (2%)	60	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	29	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	25	ASN
1	B	201	LEU
1	B	320	GLU
1	B	330	CYS
1	B	360	ILE
1	C	25	ASN
1	C	29	ILE
1	C	140	ILE
1	C	201	LEU
1	C	224	ILE
1	C	320	GLU
1	C	330	CYS

Some 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	251	GLN
1	B	174	GLN
1	B	251	GLN
1	C	25	ASN

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Mol	Chain	Res	Type
1	C	251	GLN

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	363/388 (93%)	0.30	22 (6%)	25 17	88, 195, 325, 398	0
1	B	363/388 (93%)	0.40	28 (7%)	16 12	111, 194, 317, 465	0
1	C	363/388 (93%)	0.46	32 (8%)	12 9	132, 230, 315, 427	0
All	All	1089/1164 (93%)	0.39	82 (7%)	17 13	88, 208, 320, 465	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	328	GLY	5.1
1	A	193	ARG	4.8
1	A	222	GLN	4.7
1	C	173	TRP	4.7
1	A	252	PHE	4.6
1	A	173	TRP	4.6
1	C	222	GLN	4.5
1	C	157	GLY	4.3
1	B	153	ASP	4.1
1	C	252	PHE	4.1
1	C	191	MET	4.1
1	B	288	ALA	4.0
1	B	245	GLY	4.0
1	B	246	ASP	4.0
1	C	318	ARG	3.9
1	B	277	TRP	3.8
1	C	145	TRP	3.8
1	B	397	VAL	3.7
1	A	171	LYS	3.6
1	A	157	GLY	3.4
1	C	190	GLU	3.4
1	C	356	LEU	3.4
1	A	275	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	54	SER	3.3
1	B	276	ARG	3.3
1	C	383	PRO	3.2
1	C	397	VAL	3.2
1	B	280	LEU	3.0
1	C	156	ARG	3.0
1	A	172	LYS	2.9
1	B	361	LYS	2.9
1	C	187	LYS	2.9
1	C	60	PRO	2.8
1	B	204	GLU	2.8
1	A	277	TRP	2.8
1	A	190	GLU	2.8
1	C	155	ASP	2.7
1	C	320	GLU	2.7
1	C	193	ARG	2.7
1	B	185	ASN	2.6
1	B	287	GLY	2.6
1	A	291	THR	2.6
1	A	384	ARG	2.5
1	B	222	GLN	2.5
1	C	396	VAL	2.5
1	C	119	ASP	2.5
1	A	288	ALA	2.5
1	A	395	MET	2.5
1	B	86	TYR	2.5
1	A	155	ASP	2.5
1	C	81	PHE	2.5
1	C	315	ARG	2.4
1	A	378	LEU	2.4
1	B	184	ASN	2.4
1	B	235	TYR	2.4
1	C	206	ARG	2.4
1	A	145	TRP	2.4
1	A	321	ILE	2.4
1	C	357	SER	2.3
1	B	289	HIS	2.3
1	C	86	TYR	2.3
1	A	398	THR	2.3
1	C	321	ILE	2.3
1	A	397	VAL	2.2
1	B	206	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	379	LYS	2.2
1	B	278	SER	2.2
1	B	155	ASP	2.2
1	C	194	SER	2.1
1	C	319	ILE	2.1
1	B	285	TYR	2.1
1	C	377	GLU	2.1
1	B	369	ILE	2.1
1	B	211	CYS	2.1
1	B	212	GLU	2.1
1	C	386	ILE	2.1
1	C	195	LEU	2.1
1	C	235	TYR	2.1
1	B	336	VAL	2.1
1	B	356	LEU	2.0
1	A	250	ILE	2.0
1	B	200	GLU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.