Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:49 pm BST

PDB ID	:	1J8F
Title	:	HUMAN SIRT2 HISTONE DEACETYLASE
Authors	:	Pavletich, N.P.; Finnin, M.S.; Donigian, J.R.
Deposited on	:	2001-05-21
Resolution	:	1.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

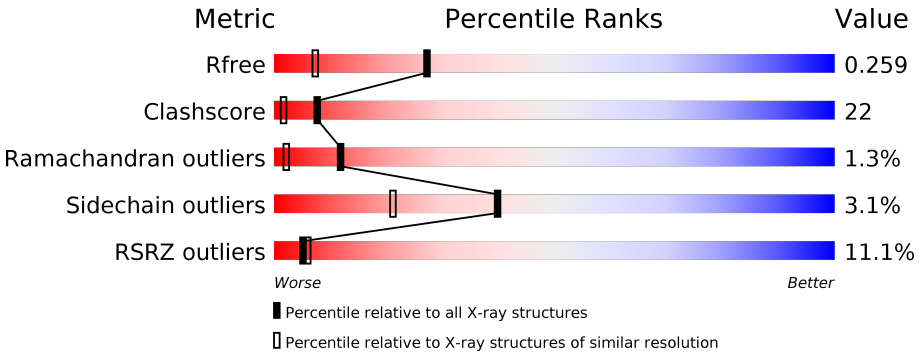
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	323	10% 67% 27%
1	B	323	14% 61% 33%
1	C	323	8% 67% 24% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11519 atoms, of which 3295 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 SIRTUIN 2, ISOFORM 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	H	N	O	S	0	0	0
			3006	1590	527	411	458	20			
1	B	312	Total	C	H	N	O	S	0	0	0
			3007	1590	527	411	459	20			
1	C	303	Total	C	H	N	O	S	0	0	0
			2905	1536	509	398	443	19			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

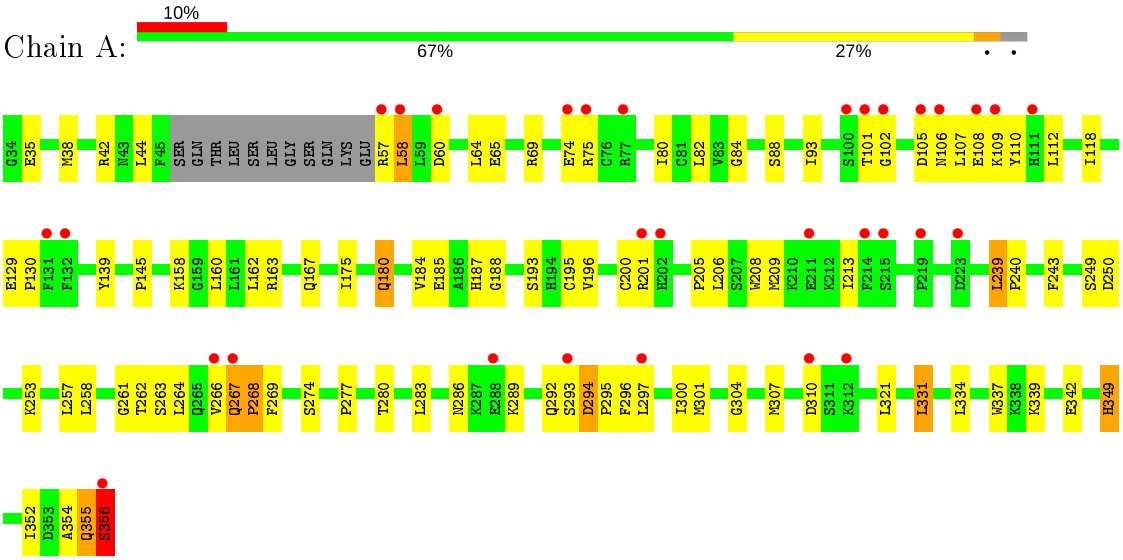
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	275	Total	H	O	0	0
			825	550	275		
3	B	276	Total	H	O	0	0
			828	552	276		
3	C	315	Total	H	O	0	0
			945	630	315		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

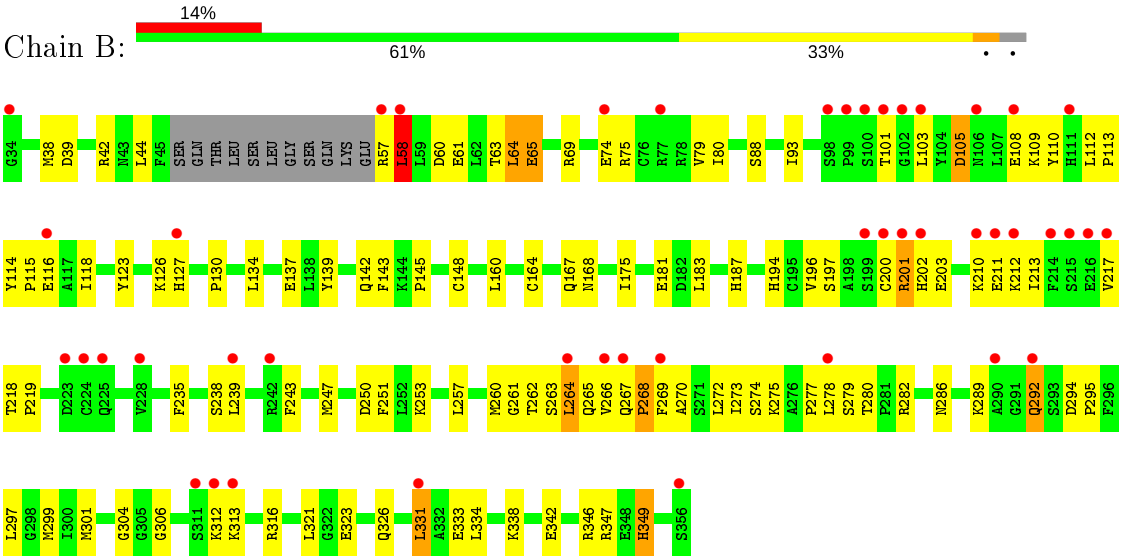
- Molecule 1: SIRTUIN 2, ISOFORM 1

Chain A:



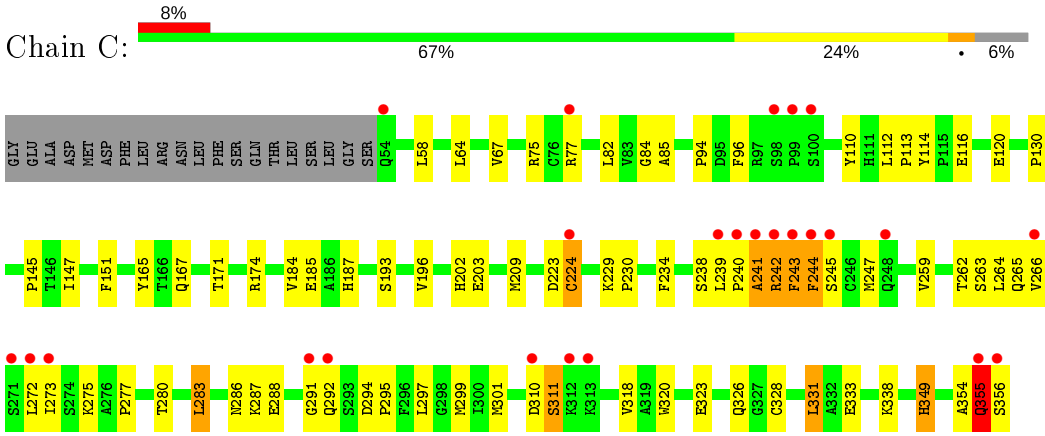
- Molecule 1: SIRTUIN 2, ISOFORM 1

Chain B:



- Molecule 1: SIRTUIN 2, ISOFORM 1

Chain C:


8%
67%
24%
6%
GLY GLU ALA ASP MET ASP PHE LEU ARG ASN LEU PHE SER GLN THR LEU SER LEU GLY SER Q54 L58 L64 V67 R75 C76 R77 L82 V83 G84 A85 P94 D95 F96 R97 S98 P99 S100 Y110 H111 L112 P113 Y114 P115 E116 E120 P130 L134 P140
P145 T146 I147 F151 Y165 T166 Q167 T171 R174 V184 E185 A186 H187 S193 V196 H202 E203 M209 D223 C224 K229 P230 F234 S238 L239 P240 A241 R242 F243 F244 S245 C246 M247 Q248 V259 T262 S263 L264 Q265 V266 Q267 P268 F269 A270
S271 L272 I273 S274 K275 A276 P277 T280 L283 N286 K287 E288 G291 Q292 S293 D294 P295 F296 L297 G298 M299 I300 M301 D310 S311 K312 K313 V318 A319 W320 E323 Q326 G327 C328 L331 A332 E333 K338 H349 A354 Q365 S356

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	78.94Å 119.07Å 218.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.70 19.90 – 1.63	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.70) 95.9 (19.90-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 1.63Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.260 0.227 , 0.259	Depositor DCC
R_{free} test set	2441 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11519	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.55	2/2536 (0.1%)	0.75	2/3420 (0.1%)
1	B	0.46	0/2537	0.79	2/3420 (0.1%)
1	C	0.48	0/2452	0.76	0/3309
All	All	0.50	2/7525 (0.0%)	0.76	4/10149 (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	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	SER	CB-OG	-12.80	1.25	1.42
1	A	356	SER	C-O	9.97	1.42	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	264	LEU	CA-CB-CG	7.60	132.77	115.30
1	B	58	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	356	SER	N-CA-CB	5.14	118.21	110.50
1	A	310	ASP	N-CA-C	5.09	124.76	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	356	SER	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2479	527	2455	105	9
1	B	2480	527	2455	135	1
1	C	2396	509	2372	84	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	275	550	0	27	11
3	B	276	552	0	38	3
3	C	315	630	0	26	7
All	All	8224	3295	7282	320	20

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 22.

All (320) 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:B:64:LEU:HD12	1:B:334:LEU:HD12	1.34	1.07
1:B:118:ILE:HD11	1:B:134:LEU:HD22	1.35	1.03
1:A:257:LEU:HD22	3:A:1205:HOH:O	1.66	0.95
1:B:200:CYS:O	1:B:201:ARG:HD3	1.67	0.95
1:B:118:ILE:HD11	1:B:134:LEU:CD2	1.96	0.94
1:A:38:MET:HB3	1:A:356:SER:HB3	1.52	0.92
1:C:292:GLN:HA	3:C:3297:HOH:O	1.70	0.91
1:C:151:PHE:HB2	3:C:3278:HOH:O	1.70	0.90
1:A:167:GLN:HB3	3:A:1208:HOH:O	1.72	0.89
1:B:210:LYS:HG3	3:B:2201:HOH:O	1.74	0.87
1:A:162:LEU:HG	3:A:1262:HOH:O	1.73	0.87
1:B:301:MET:HG3	3:B:2159:HOH:O	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:PRO:HG2	1:B:280:THR:OG1	1.79	0.83
1:A:266:VAL:HB	3:A:1151:HOH:O	1.78	0.83
1:C:354:ALA:O	1:C:355:GLN:HB2	1.79	0.82
1:A:38:MET:HB3	1:A:356:SER:CB	2.09	0.82
1:A:74:GLU:OE2	1:A:75:ARG:HG2	1.82	0.80
1:B:262:THR:HG22	1:B:263:SER:H	1.47	0.80
1:C:294:ASP:CG	1:C:297:LEU:HD13	2.02	0.79
1:B:200:CYS:C	1:B:201:ARG:HD3	2.02	0.79
1:B:313:LYS:HE3	3:B:2110:HOH:O	1.82	0.79
1:C:239:LEU:HD12	1:C:239:LEU:H	1.47	0.79
1:B:118:ILE:CD1	1:B:134:LEU:HD22	2.11	0.79
1:B:64:LEU:HD12	1:B:334:LEU:CD1	2.12	0.79
1:A:167:GLN:HG3	3:A:1140:HOH:O	1.83	0.77
1:A:38:MET:HE2	1:A:356:SER:CB	2.17	0.75
1:C:277:PRO:HG2	1:C:280:THR:OG1	1.87	0.75
1:A:38:MET:HE2	1:A:356:SER:HB3	1.67	0.75
1:B:273:ILE:HG23	3:B:2207:HOH:O	1.86	0.74
1:A:266:VAL:HG22	1:A:268:PRO:HD2	1.69	0.74
1:B:112:LEU:HD13	3:B:2140:HOH:O	1.86	0.74
1:B:316:ARG:HD3	3:B:2269:HOH:O	1.87	0.74
1:B:103:LEU:HB2	3:B:2176:HOH:O	1.86	0.74
1:C:94:PRO:HG2	1:C:96:PHE:CZ	2.22	0.73
1:B:264:LEU:HD12	3:B:2108:HOH:O	1.89	0.72
1:A:263:SER:HB3	3:A:1151:HOH:O	1.89	0.72
1:C:209:MET:SD	3:C:3114:HOH:O	2.49	0.71
1:B:115:PRO:O	1:B:118:ILE:HG22	1.90	0.71
1:C:243:PHE:HB3	1:C:247:MET:HE3	1.72	0.71
1:A:107:LEU:HD13	3:A:1231:HOH:O	1.91	0.70
1:A:267:GLN:O	3:A:1252:HOH:O	2.10	0.70
1:C:287:LYS:HE2	1:C:323:GLU:OE2	1.91	0.70
1:A:184:VAL:HG22	3:A:1266:HOH:O	1.91	0.70
1:A:69:ARG:HD2	1:B:58:LEU:HG	1.73	0.70
1:C:174:ARG:NH1	1:C:185:GLU:OE2	2.22	0.70
1:B:263:SER:O	1:B:264:LEU:HB2	1.92	0.70
1:A:277:PRO:HG2	1:A:280:THR:OG1	1.92	0.69
1:B:57:ARG:HG2	1:B:75:ARG:NH1	2.07	0.69
1:B:167:GLN:HE22	1:B:262:THR:HG23	1.55	0.69
1:B:118:ILE:HG13	3:B:2084:HOH:O	1.93	0.68
1:C:58:LEU:HD22	1:C:75:ARG:HE	1.57	0.68
1:B:57:ARG:N	1:B:75:ARG:HH11	1.90	0.68
1:C:273:ILE:HA	3:C:3286:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:PRO:HA	3:C:3220:HOH:O	1.93	0.68
1:B:210:LYS:HD2	1:B:210:LYS:O	1.94	0.67
1:B:57:ARG:HD3	1:B:75:ARG:HD3	1.75	0.67
1:A:268:PRO:HG2	1:A:269:PHE:H	1.59	0.67
1:B:116:GLU:HG3	1:B:235:PHE:CE1	2.29	0.67
1:C:240:PRO:O	1:C:241:ALA:HB3	1.96	0.66
1:B:347:ARG:HD3	3:B:2079:HOH:O	1.94	0.66
1:B:261:GLY:HA2	1:B:286:ASN:ND2	2.11	0.66
1:A:297:LEU:O	1:A:301:MET:HG3	1.95	0.65
1:B:105:ASP:O	1:B:108:GLU:HG3	1.96	0.65
1:B:167:GLN:NE2	1:B:262:THR:HG23	2.12	0.65
1:A:57:ARG:HH11	1:A:75:ARG:HB3	1.59	0.65
1:C:238:SER:HB3	3:C:3213:HOH:O	1.96	0.65
1:A:187:HIS:HD2	3:A:1014:HOH:O	1.80	0.64
1:C:82:LEU:HD23	1:C:165:TYR:HB2	1.79	0.64
1:C:263:SER:O	1:C:266:VAL:HG12	1.96	0.64
1:C:239:LEU:CD1	1:C:239:LEU:H	2.10	0.63
1:A:195:CYS:O	1:A:201:ARG:NH2	2.30	0.63
1:A:42:ARG:HH22	1:A:356:SER:HA	1.63	0.63
1:C:310:ASP:O	1:C:311:SER:HB2	1.98	0.62
1:C:239:LEU:N	1:C:239:LEU:HD12	2.14	0.62
1:B:294:ASP:CG	1:B:297:LEU:HD13	2.20	0.62
1:B:103:LEU:HD22	1:B:137:GLU:OE2	1.99	0.62
1:B:168:ASN:ND2	3:B:2003:HOH:O	2.33	0.61
1:B:266:VAL:HG12	3:B:2160:HOH:O	2.00	0.61
1:C:333:GLU:HB2	1:C:338:LYS:HE3	1.80	0.61
1:C:243:PHE:HB3	1:C:247:MET:CE	2.30	0.61
1:C:134:LEU:HD23	1:C:134:LEU:C	2.21	0.61
1:C:147:ILE:HG22	3:C:3278:HOH:O	1.99	0.61
1:C:270:ALA:HA	1:C:273:ILE:HD12	1.82	0.61
1:B:264:LEU:HD22	1:B:273:ILE:HD13	1.81	0.61
1:C:320:TRP:HB2	3:C:3273:HOH:O	2.00	0.60
1:C:116:GLU:O	1:C:120:GLU:HG3	2.00	0.60
1:C:264:LEU:CD2	1:C:273:ILE:HD13	2.32	0.60
1:A:185:GLU:HB2	3:A:1227:HOH:O	2.00	0.60
1:C:291:GLY:O	3:C:3252:HOH:O	2.16	0.59
1:C:209:MET:CE	3:C:3114:HOH:O	2.50	0.59
1:A:158:LYS:HB2	1:A:160:LEU:HD23	1.83	0.59
1:A:88:SER:HB3	1:A:93:ILE:HG13	1.84	0.59
1:B:210:LYS:HD2	1:B:210:LYS:C	2.22	0.59
1:C:287:LYS:HE2	1:C:323:GLU:CD	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:HIS:HD2	3:C:3010:HOH:O	1.85	0.58
1:C:291:GLY:C	3:C:3252:HOH:O	2.41	0.58
1:B:266:VAL:CG1	3:B:2160:HOH:O	2.51	0.58
1:A:102:GLY:HA2	1:A:105:ASP:OD1	2.03	0.58
1:B:197:SER:OG	1:B:200:CYS:HB3	2.03	0.58
1:B:263:SER:O	1:B:264:LEU:CB	2.48	0.58
1:C:265:GLN:HG3	1:C:301:MET:CE	2.33	0.58
1:B:262:THR:HG22	1:B:263:SER:N	2.18	0.57
1:B:264:LEU:CD2	1:B:273:ILE:HD13	2.33	0.57
1:B:338:LYS:O	1:B:342:GLU:HG3	2.05	0.57
1:B:60:ASP:OD2	1:B:69:ARG:HD2	2.04	0.57
1:A:42:ARG:NH2	1:A:356:SER:HA	2.21	0.56
1:B:39:ASP:OD1	1:B:42:ARG:NH2	2.36	0.56
1:B:64:LEU:HD11	1:B:331:LEU:HA	1.88	0.56
1:C:242:ARG:HG2	1:C:242:ARG:HH11	1.71	0.56
1:A:249:SER:O	1:A:253:LYS:HE3	2.06	0.56
1:A:274:SER:HB2	1:A:304:GLY:O	2.06	0.56
1:A:294:ASP:OD2	1:A:297:LEU:HD13	2.06	0.56
1:B:292:GLN:CD	1:B:292:GLN:H	2.09	0.56
1:A:80:ILE:HD11	1:A:250:ASP:HB3	1.88	0.55
1:B:253:LYS:HD3	3:B:2202:HOH:O	2.06	0.55
1:A:239:LEU:HD13	3:A:1031:HOH:O	2.06	0.55
1:A:69:ARG:CD	1:B:58:LEU:HG	2.37	0.55
1:B:263:SER:O	3:B:2083:HOH:O	2.18	0.55
1:A:42:ARG:HH12	1:A:356:SER:HB2	1.72	0.55
1:B:148:CYS:SG	3:B:2002:HOH:O	2.53	0.55
1:C:272:LEU:HA	1:C:275:LYS:HE3	1.88	0.55
1:A:205:PRO:HG2	1:A:208:TRP:HB2	1.90	0.54
1:B:247:MET:HG3	1:B:272:LEU:CD2	2.37	0.54
1:C:243:PHE:O	1:C:245:SER:N	2.40	0.54
1:A:139:TYR:CE2	1:A:213:ILE:CD1	2.91	0.54
1:B:57:ARG:N	1:B:75:ARG:NH1	2.55	0.54
1:B:262:THR:HG21	1:B:269:PHE:HD2	1.73	0.54
1:B:333:GLU:OE2	1:B:338:LYS:HG3	2.07	0.54
1:A:354:ALA:O	1:A:355:GLN:HB2	2.08	0.54
1:B:116:GLU:HG3	1:B:235:PHE:CD1	2.42	0.54
1:C:112:LEU:HD13	3:C:3309:HOH:O	2.07	0.53
1:C:287:LYS:HE2	1:C:323:GLU:OE1	2.09	0.53
1:B:126:LYS:HG3	1:B:127:HIS:ND1	2.24	0.53
1:B:295:PRO:O	1:B:299:MET:HG3	2.09	0.53
1:C:230:PRO:HB3	3:C:3012:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:O	1:A:109:LYS:HE3	2.08	0.53
1:B:201:ARG:HG2	1:B:201:ARG:O	2.09	0.53
1:C:240:PRO:O	1:C:241:ALA:CB	2.56	0.53
1:B:38:MET:HE2	1:B:38:MET:HA	1.91	0.53
1:B:44:LEU:HD13	1:B:175:ILE:HG12	1.91	0.53
1:A:44:LEU:HD13	1:A:175:ILE:HG12	1.90	0.53
1:C:113:PRO:HB2	1:C:114:TYR:CD2	2.44	0.52
1:A:180:GLN:HE21	1:A:180:GLN:HA	1.75	0.52
1:C:264:LEU:HD22	1:C:273:ILE:HD13	1.90	0.52
1:B:142:GLN:HB2	3:B:2231:HOH:O	2.10	0.52
1:B:274:SER:HB3	3:B:2163:HOH:O	2.09	0.52
1:A:293:SER:O	1:A:294:ASP:HB2	2.10	0.52
1:B:57:ARG:CD	1:B:75:ARG:HD3	2.40	0.52
1:A:167:GLN:HE21	1:A:266:VAL:HG21	1.75	0.51
1:A:38:MET:HB3	1:A:356:SER:OG	2.10	0.51
1:B:88:SER:HB3	1:B:93:ILE:HG13	1.93	0.51
1:B:187:HIS:HD2	3:B:2025:HOH:O	1.93	0.51
1:B:202:HIS:HD2	1:B:203:GLU:N	2.09	0.51
1:A:105:ASP:HB2	3:A:1055:HOH:O	2.09	0.51
1:A:58:LEU:HB3	3:A:1146:HOH:O	2.10	0.51
1:B:278:LEU:H	1:B:278:LEU:HD22	1.75	0.51
1:A:129:GLU:CD	1:A:129:GLU:H	2.14	0.51
1:C:223:ASP:HB2	1:C:224:CYS:SG	2.50	0.51
1:B:251:PHE:O	1:B:277:PRO:HD3	2.11	0.51
1:B:239:LEU:HD12	1:B:239:LEU:H	1.76	0.51
1:B:64:LEU:O	1:B:64:LEU:HD13	2.11	0.51
1:A:57:ARG:HD2	3:A:1059:HOH:O	2.10	0.50
1:B:64:LEU:HD11	1:B:331:LEU:HG	1.93	0.50
1:A:110:TYR:CG	1:A:130:PRO:HG3	2.47	0.50
1:C:356:SER:HB3	3:C:3113:HOH:O	2.11	0.50
1:A:240:PRO:HG2	1:A:243:PHE:CD1	2.46	0.50
1:C:238:SER:CB	3:C:3213:HOH:O	2.55	0.50
1:C:196:VAL:HG12	1:C:229:LYS:HG2	1.94	0.50
1:C:264:LEU:O	1:C:273:ILE:HD12	2.12	0.49
1:C:288:GLU:HB3	3:C:3222:HOH:O	2.12	0.49
1:A:109:LYS:HD2	3:A:1129:HOH:O	2.13	0.49
1:A:167:GLN:NE2	1:A:268:PRO:HG3	2.27	0.49
1:A:188:GLY:HA2	3:A:1227:HOH:O	2.12	0.49
1:B:196:VAL:HG12	1:B:196:VAL:O	2.13	0.49
1:B:80:ILE:HD11	1:B:250:ASP:HB3	1.95	0.49
1:C:243:PHE:O	1:C:244:PHE:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:O	1:A:109:LYS:N	2.40	0.49
1:B:278:LEU:N	1:B:278:LEU:HD22	2.28	0.49
1:B:279:SER:HA	3:B:2269:HOH:O	2.12	0.49
1:B:260:MET:HE3	3:B:2002:HOH:O	2.12	0.49
1:C:110:TYR:HB3	1:C:130:PRO:HG3	1.94	0.49
1:A:106:ASN:HA	1:A:109:LYS:HE3	1.95	0.48
1:A:139:TYR:CE2	1:A:213:ILE:HD13	2.48	0.48
1:A:64:LEU:HD11	1:A:331:LEU:HG	1.95	0.48
1:A:112:LEU:N	1:A:112:LEU:HD22	2.28	0.48
1:A:35:GLU:HG3	3:A:1110:HOH:O	2.13	0.48
1:B:65:GLU:OE1	1:B:69:ARG:CZ	2.61	0.48
1:C:355:GLN:HB2	3:C:3223:HOH:O	2.13	0.48
1:B:306:GLY:HA2	3:B:2163:HOH:O	2.12	0.48
1:A:163:ARG:CZ	3:A:1262:HOH:O	2.61	0.48
1:B:194:HIS:CD2	1:B:203:GLU:HB2	2.48	0.48
1:B:286:ASN:ND2	3:B:2182:HOH:O	2.46	0.48
1:C:328:CYS:HB3	3:C:3278:HOH:O	2.14	0.48
1:C:318:VAL:HG12	3:C:3273:HOH:O	2.14	0.48
1:C:269:PHE:HD2	3:C:3158:HOH:O	1.96	0.48
1:C:326:GLN:NE2	3:C:3149:HOH:O	2.46	0.48
1:A:145:PRO:O	1:A:349:HIS:HE1	1.97	0.47
1:B:292:GLN:NE2	1:B:292:GLN:N	2.61	0.47
1:C:355:GLN:OE1	1:C:355:GLN:HA	2.14	0.47
1:B:118:ILE:CG1	3:B:2084:HOH:O	2.58	0.47
1:B:113:PRO:HB2	1:B:114:TYR:CD2	2.48	0.47
1:B:247:MET:HG3	1:B:272:LEU:HD21	1.96	0.47
1:B:61:GLU:HG3	1:B:63:THR:OG1	2.14	0.47
1:C:295:PRO:O	1:C:299:MET:HG3	2.14	0.47
1:B:264:LEU:HD23	1:B:273:ILE:CD1	2.45	0.47
1:B:118:ILE:HD11	1:B:134:LEU:HD23	1.88	0.47
1:B:181:GLU:H	1:B:181:GLU:CD	2.18	0.47
1:C:77:ARG:HG2	1:C:77:ARG:HH11	1.80	0.47
1:B:103:LEU:HD12	3:B:2176:HOH:O	2.13	0.47
1:B:263:SER:OG	1:B:265:GLN:HB3	2.14	0.47
1:A:82:LEU:HG	3:A:1205:HOH:O	2.15	0.46
1:A:108:GLU:C	1:A:109:LYS:HG3	2.35	0.46
1:B:101:THR:N	3:B:2128:HOH:O	2.47	0.46
1:C:264:LEU:HD22	1:C:273:ILE:HG21	1.96	0.46
1:B:349:HIS:HD2	3:B:2135:HOH:O	1.98	0.46
1:C:184:VAL:HA	1:C:243:PHE:CE1	2.51	0.46
1:C:58:LEU:HD22	1:C:75:ARG:NE	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:H	1:B:74:GLU:CD	2.18	0.46
1:A:158:LYS:CB	1:A:160:LEU:HD23	2.46	0.46
1:B:260:MET:CE	3:B:2002:HOH:O	2.63	0.46
1:C:145:PRO:O	1:C:349:HIS:HE1	1.98	0.46
1:C:294:ASP:OD1	1:C:297:LEU:HD13	2.14	0.46
1:A:118:ILE:HD12	3:A:1231:HOH:O	2.15	0.46
1:B:278:LEU:H	1:B:278:LEU:CD2	2.28	0.46
1:B:282:ARG:HD2	3:B:2207:HOH:O	2.16	0.46
1:A:261:GLY:HA2	1:A:286:ASN:ND2	2.31	0.45
1:B:247:MET:SD	1:B:275:LYS:NZ	2.85	0.45
1:B:79:VAL:HG23	3:B:2204:HOH:O	2.15	0.45
1:A:57:ARG:NH1	1:A:75:ARG:HB3	2.30	0.45
1:C:64:LEU:HD11	1:C:331:LEU:HG	1.98	0.45
1:A:240:PRO:HG2	1:A:243:PHE:CE1	2.51	0.45
1:A:264:LEU:HD13	1:A:307:MET:HG3	1.99	0.45
1:B:239:LEU:N	1:B:239:LEU:HD12	2.32	0.45
1:A:268:PRO:HG2	1:A:269:PHE:N	2.29	0.45
1:B:292:GLN:NE2	1:B:292:GLN:H	2.15	0.45
1:C:202:HIS:HD2	1:C:203:GLU:N	2.14	0.45
1:B:139:TYR:CE2	1:B:213:ILE:CD1	3.00	0.45
1:A:352:ILE:O	1:A:355:GLN:OE1	2.35	0.45
1:A:57:ARG:HD3	1:A:75:ARG:NE	2.31	0.45
1:B:266:VAL:O	1:B:268:PRO:HD2	2.17	0.45
1:C:294:ASP:OD2	1:C:297:LEU:HD13	2.17	0.45
1:A:129:GLU:HB2	1:A:130:PRO:HD3	1.98	0.44
1:B:238:SER:HA	3:B:2093:HOH:O	2.17	0.44
1:A:110:TYR:CD2	1:A:130:PRO:HG3	2.53	0.44
1:A:243:PHE:HZ	3:A:1227:HOH:O	1.99	0.44
1:B:110:TYR:CG	1:B:130:PRO:HG3	2.51	0.44
1:B:257:LEU:HD23	3:B:2207:HOH:O	2.16	0.44
1:A:355:GLN:O	1:A:356:SER:OG	2.23	0.44
1:A:57:ARG:HD3	1:A:75:ARG:HE	1.83	0.44
1:B:289:LYS:HG3	1:B:321:LEU:HD21	1.99	0.44
1:B:109:LYS:HE3	3:B:2241:HOH:O	2.17	0.44
1:A:193:SER:OG	1:A:209:MET:HG3	2.18	0.44
1:B:218:THR:HA	1:B:219:PRO:HD3	1.91	0.43
1:A:84:GLY:HA3	1:A:262:THR:HB	2.01	0.43
1:A:339:LYS:O	1:A:342:GLU:HB3	2.18	0.43
1:B:101:THR:CG2	3:B:2116:HOH:O	2.66	0.43
1:C:112:LEU:HA	1:C:113:PRO:HD3	1.87	0.43
1:C:147:ILE:CG2	3:C:3278:HOH:O	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:GLY:HA3	1:C:262:THR:HB	1.99	0.43
1:B:167:GLN:HG3	1:B:269:PHE:CE2	2.53	0.43
1:C:310:ASP:O	1:C:311:SER:CB	2.66	0.43
1:A:38:MET:CB	1:A:356:SER:HB3	2.36	0.43
1:B:262:THR:HG21	1:B:269:PHE:CD2	2.52	0.43
1:C:229:LYS:HE3	1:C:234:PHE:CD1	2.54	0.43
1:B:239:LEU:HD23	1:B:243:PHE:HD2	1.84	0.43
1:C:67:VAL:HG21	1:C:283:LEU:HG	2.00	0.43
1:A:60:ASP:HB3	1:B:57:ARG:N	2.34	0.42
1:B:212:LYS:HB3	1:B:217:VAL:O	2.19	0.42
1:B:274:SER:HB2	1:B:304:GLY:O	2.19	0.42
1:B:93:ILE:HD13	1:B:143:PHE:CD1	2.54	0.42
1:C:174:ARG:HH11	1:C:174:ARG:HG3	1.83	0.42
1:A:163:ARG:NE	3:A:1262:HOH:O	2.51	0.42
1:B:164:CYS:HB3	1:B:183:LEU:HD23	2.02	0.42
1:A:101:THR:HB	3:A:1061:HOH:O	2.19	0.42
1:A:266:VAL:CG1	1:A:269:PHE:HB2	2.50	0.42
1:C:229:LYS:HE3	1:C:234:PHE:CE1	2.54	0.42
1:B:123:TYR:O	1:B:126:LYS:HG2	2.19	0.42
1:C:209:MET:HE1	3:C:3114:HOH:O	2.17	0.42
1:A:57:ARG:HG2	1:A:75:ARG:NH2	2.35	0.42
1:B:275:LYS:HE3	1:B:275:LYS:HB2	1.91	0.42
1:B:292:GLN:CA	1:B:292:GLN:HE21	2.32	0.42
1:A:286:ASN:O	1:A:321:LEU:HA	2.18	0.42
1:A:196:VAL:HA	1:A:201:ARG:HH21	1.85	0.42
1:A:163:ARG:HB2	3:A:1262:HOH:O	2.18	0.41
1:A:267:GLN:N	3:A:1198:HOH:O	2.49	0.41
1:A:258:LEU:HD22	1:A:283:LEU:HD23	2.02	0.41
1:A:158:LYS:HE3	1:A:337:TRP:CE2	2.55	0.41
1:B:239:LEU:CD1	1:B:239:LEU:H	2.33	0.41
1:C:202:HIS:HB2	3:C:3175:HOH:O	2.19	0.41
1:C:82:LEU:HD12	1:C:259:VAL:HG22	2.02	0.41
1:B:110:TYR:CD2	1:B:130:PRO:HG3	2.55	0.41
1:A:266:VAL:HG11	1:A:269:PHE:CD2	2.55	0.41
1:B:101:THR:HG21	3:B:2116:HOH:O	2.20	0.41
1:C:265:GLN:HG3	1:C:301:MET:SD	2.61	0.41
1:A:69:ARG:HD2	1:B:58:LEU:CG	2.47	0.41
1:A:289:LYS:HG3	1:A:321:LEU:HD21	2.03	0.41
1:A:294:ASP:HA	1:A:295:PRO:HD3	1.67	0.41
1:C:193:SER:OG	1:C:209:MET:HG3	2.20	0.41
1:A:296:PHE:O	1:A:300:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLU:HA	1:A:334:LEU:HD13	2.03	0.41
1:B:266:VAL:HG22	1:B:268:PRO:HD2	2.03	0.41
1:A:266:VAL:HG11	1:A:269:PHE:HD2	1.85	0.41
1:B:160:LEU:HD22	3:B:2204:HOH:O	2.21	0.41
1:B:268:PRO:HA	3:B:2218:HOH:O	2.20	0.41
1:B:294:ASP:OD1	1:B:297:LEU:HD13	2.19	0.41
1:B:202:HIS:CD2	1:B:203:GLU:N	2.87	0.41
1:B:269:PHE:O	1:B:270:ALA:C	2.58	0.41
1:B:65:GLU:HB2	3:B:2054:HOH:O	2.21	0.41
1:C:167:GLN:HB2	1:C:167:GLN:HE21	1.64	0.41
1:B:145:PRO:O	1:B:349:HIS:HE1	2.04	0.41
1:A:200:CYS:O	1:A:201:ARG:HB2	2.20	0.40
1:B:323:GLU:HB2	1:B:326:GLN:HG2	2.04	0.40
1:C:114:TYR:HE1	1:C:120:GLU:CD	2.25	0.40
1:A:206:LEU:HD13	1:A:206:LEU:C	2.42	0.40
1:A:267:GLN:HB3	1:A:268:PRO:CD	2.51	0.40
1:A:267:GLN:HB3	1:A:268:PRO:HD3	2.04	0.40
1:A:293:SER:O	1:A:294:ASP:CB	2.69	0.40
1:B:181:GLU:N	1:B:181:GLU:CD	2.74	0.40
1:A:58:LEU:HB2	3:A:1130:HOH:O	2.21	0.40
1:C:171:THR:HB	3:C:3220:HOH:O	2.20	0.40

All (20) 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:A:293:SER:HG	1:C:85:ALA:H[8_455]	0.18	1.42
1:A:339:LYS:HZ3	3:A:1160:HOH:H2[3_655]	0.65	0.95
1:A:339:LYS:NZ	3:A:1160:HOH:H2[3_655]	0.80	0.80
1:A:339:LYS:NZ	3:A:1160:HOH:H1[3_655]	0.90	0.70
1:A:293:SER:HG	1:C:85:ALA:N[8_455]	0.91	0.69
1:A:339:LYS:HZ2	3:A:1160:HOH:H1[3_655]	0.98	0.62
3:C:3313:HOH:H2	3:C:3314:HOH:O[4_565]	1.01	0.59
3:C:3181:HOH:H1	3:C:3195:HOH:H1[4_555]	1.10	0.50
3:C:3313:HOH:O	3:C:3313:HOH:O[4_565]	1.77	0.43
3:C:3072:HOH:O	3:C:3072:HOH:O[4_565]	1.77	0.43
3:A:1137:HOH:H2	3:B:2117:HOH:H1[1_455]	1.19	0.41
3:A:1046:HOH:H2	3:B:2264:HOH:H1[1_455]	1.27	0.33
3:C:3141:HOH:H2	3:C:3195:HOH:H2[4_555]	1.31	0.29
1:B:346:ARG:HH22	3:A:1048:HOH:H2[1_655]	1.34	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3313:HOH:H1	3:C:3314:HOH:O[4_565]	1.36	0.24
1:A:339:LYS:CE	3:A:1160:HOH:H1[3_655]	1.40	0.20
1:A:339:LYS:CE	3:A:1160:HOH:H2[3_655]	1.44	0.16
1:A:339:LYS:HZ1	3:A:1081:HOH:O[3_655]	1.49	0.11
3:A:1137:HOH:O	3:B:2117:HOH:H1[1_455]	1.58	0.02
3:C:3181:HOH:H1	3:C:3195:HOH:O[4_555]	1.59	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	308/323 (95%)	292 (95%)	12 (4%)	4 (1%)	12 2
1	B	308/323 (95%)	294 (96%)	11 (4%)	3 (1%)	15 4
1	C	301/323 (93%)	287 (95%)	9 (3%)	5 (2%)	9 1
All	All	917/969 (95%)	873 (95%)	32 (4%)	12 (1%)	12 2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	GLN
1	A	294	ASP
1	C	355	GLN
1	B	312	LYS
1	C	241	ALA
1	C	243	PHE
1	C	244	PHE
1	C	311	SER
1	B	268	PRO
1	B	267	GLN
1	A	268	PRO
1	A	267	GLN

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	271/281 (96%)	264 (97%)	7 (3%)	46	28
1	B	271/281 (96%)	262 (97%)	9 (3%)	38	19
1	C	261/281 (93%)	252 (97%)	9 (3%)	37	18
All	All	803/843 (95%)	778 (97%)	25 (3%)	40	21

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	180	GLN
1	A	239	LEU
1	A	331	LEU
1	A	349	HIS
1	A	355	GLN
1	A	356	SER
1	B	58	LEU
1	B	64	LEU
1	B	65	GLU
1	B	105	ASP
1	B	201	ARG
1	B	211	GLU
1	B	292	GLN
1	B	331	LEU
1	B	349	HIS
1	C	140	PRO
1	C	224	CYS
1	C	242	ARG
1	C	268	PRO
1	C	283	LEU
1	C	286	ASN
1	C	331	LEU
1	C	349	HIS
1	C	355	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	167	GLN
1	A	180	GLN
1	A	187	HIS
1	A	286	ASN
1	A	349	HIS
1	B	106	ASN
1	B	167	GLN
1	B	187	HIS
1	B	202	HIS
1	B	286	ASN
1	B	292	GLN
1	B	326	GLN
1	B	349	HIS
1	C	106	ASN
1	C	111	HIS
1	C	167	GLN
1	C	187	HIS
1	C	225	GLN
1	C	286	ASN
1	C	326	GLN
1	C	349	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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

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	312/323 (96%)	0.81	31 (9%) 7 8	8, 21, 39, 49	0
1	B	312/323 (96%)	0.93	45 (14%) 2 2	7, 20, 40, 49	0
1	C	303/323 (93%)	0.61	27 (8%) 9 11	7, 15, 40, 45	0
All	All	927/969 (95%)	0.78	103 (11%) 5 6	7, 19, 40, 49	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	PHE	11.3
1	B	100	SER	10.4
1	A	356	SER	7.6
1	C	243	PHE	7.6
1	B	267	GLN	7.5
1	B	101	THR	7.3
1	A	57	ARG	6.6
1	C	356	SER	6.6
1	A	108	GLU	5.7
1	B	214	PHE	5.6
1	B	57	ARG	5.6
1	C	224	CYS	5.6
1	B	266	VAL	5.6
1	B	201	ARG	5.6
1	A	100	SER	5.4
1	A	101	THR	5.3
1	B	102	GLY	5.3
1	A	266	VAL	5.3
1	B	99	PRO	5.3
1	C	273	ILE	4.6
1	C	248	GLN	4.6
1	A	267	GLN	4.6
1	A	105	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	75	ARG	4.3
1	C	310	ASP	4.3
1	A	293	SER	4.2
1	B	111	HIS	4.1
1	B	211	GLU	4.0
1	B	239	LEU	3.8
1	B	217	VAL	3.8
1	B	311	SER	3.8
1	B	215	SER	3.7
1	C	239	LEU	3.7
1	B	58	LEU	3.7
1	B	34	GLY	3.6
1	B	312	LYS	3.6
1	B	210	LYS	3.4
1	B	313	LYS	3.3
1	B	356	SER	3.3
1	B	103	LEU	3.3
1	A	214	PHE	3.3
1	C	312	LYS	3.3
1	A	202	HIS	3.2
1	A	74	GLU	3.1
1	A	223	ASP	3.1
1	C	266	VAL	3.1
1	C	241	ALA	3.1
1	C	245	SER	3.1
1	B	202	HIS	3.0
1	C	240	PRO	3.0
1	B	269	PHE	3.0
1	B	264	LEU	3.0
1	A	106	ASN	2.9
1	A	109	LYS	2.9
1	A	77	ARG	2.9
1	B	74	GLU	2.9
1	A	215	SER	2.8
1	A	297	LEU	2.8
1	B	242	ARG	2.8
1	B	212	LYS	2.8
1	C	99	PRO	2.8
1	C	272	LEU	2.8
1	C	271	SER	2.7
1	A	310	ASP	2.7
1	B	200	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	292	GLN	2.7
1	C	291	GLY	2.6
1	B	225	GLN	2.6
1	B	108	GLU	2.6
1	A	60	ASP	2.6
1	B	290	ALA	2.5
1	B	228	VAL	2.5
1	A	102	GLY	2.5
1	C	54	GLN	2.5
1	B	106	ASN	2.4
1	A	312	LYS	2.4
1	A	111	HIS	2.4
1	C	269	PHE	2.4
1	C	355	GLN	2.4
1	C	242	ARG	2.3
1	B	98	SER	2.3
1	B	224	CYS	2.3
1	A	219	PRO	2.3
1	B	127	HIS	2.3
1	A	131	PHE	2.2
1	C	268	PRO	2.2
1	C	292	GLN	2.2
1	B	278	LEU	2.2
1	B	116	GLU	2.2
1	C	100	SER	2.2
1	A	211	GLU	2.2
1	A	288	GLU	2.2
1	B	223	ASP	2.2
1	C	313	LYS	2.2
1	B	77	ARG	2.1
1	B	331	LEU	2.1
1	B	199	SER	2.1
1	A	201	ARG	2.1
1	A	132	PHE	2.1
1	A	58	LEU	2.1
1	C	77	ARG	2.0
1	B	216	GLU	2.0
1	C	98	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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, 95^{th} 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	ZN	B	2001	1/1	0.95	0.06	33,33,33,33	0
2	ZN	C	3001	1/1	0.97	0.06	14,14,14,14	0
2	ZN	A	1001	1/1	0.98	0.08	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.