Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2022 – 01:17 pm BST

PDB ID	:	7QXM
Title	:	Crystal structure of the Vibrio cholerae replicative helicase (DnaB)
Authors	:	Legrand, P.; Quevillon-Cheruel, S.; Walbott, H.; Cargemel, C.
Deposited on	:	2022-01-26
Resolution	:	3.80 Å(reported)

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

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

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

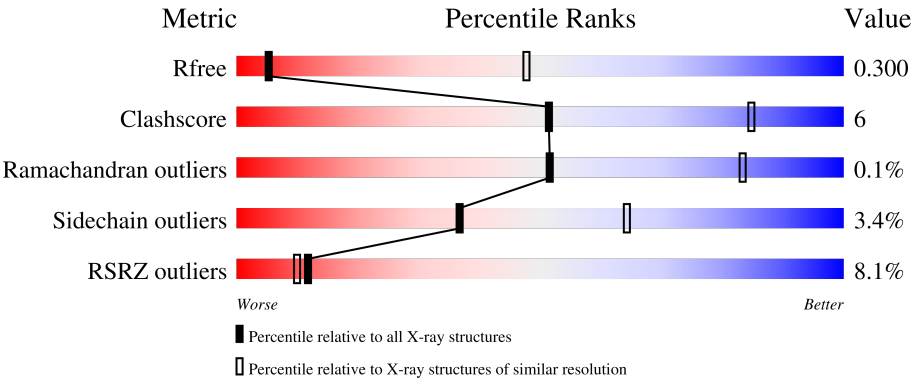
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	474	5% 79% 14% 7%
1	B	474	9% 78% 14% 7%
1	C	474	9% 79% 15% • 5%
1	D	474	8% 77% 15% 7%
1	E	474	5% 78% 15% • 6%

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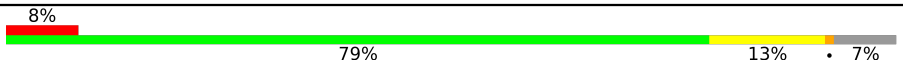
Mol	Chain	Length	Quality of chain
1	F	474	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 20679 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 Replicative DNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3433	2139	603	676	15			
1	B	440	Total	C	N	O	S	0	0	0
			3436	2142	603	676	15			
1	C	448	Total	C	N	O	S	0	0	0
			3493	2177	612	689	15			
1	D	439	Total	C	N	O	S	0	0	0
			3428	2136	602	675	15			
1	E	444	Total	C	N	O	S	0	0	0
			3460	2158	607	680	15			
1	F	440	Total	C	N	O	S	0	0	0
			3429	2136	603	675	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	HIS	-	expression tag	UNP A0A085R2T8
A	470	HIS	-	expression tag	UNP A0A085R2T8
A	471	HIS	-	expression tag	UNP A0A085R2T8
A	472	HIS	-	expression tag	UNP A0A085R2T8
A	473	HIS	-	expression tag	UNP A0A085R2T8
A	474	HIS	-	expression tag	UNP A0A085R2T8
B	469	HIS	-	expression tag	UNP A0A085R2T8
B	470	HIS	-	expression tag	UNP A0A085R2T8
B	471	HIS	-	expression tag	UNP A0A085R2T8
B	472	HIS	-	expression tag	UNP A0A085R2T8
B	473	HIS	-	expression tag	UNP A0A085R2T8
B	474	HIS	-	expression tag	UNP A0A085R2T8
C	469	HIS	-	expression tag	UNP A0A085R2T8
C	470	HIS	-	expression tag	UNP A0A085R2T8
C	471	HIS	-	expression tag	UNP A0A085R2T8
C	472	HIS	-	expression tag	UNP A0A085R2T8
C	473	HIS	-	expression tag	UNP A0A085R2T8

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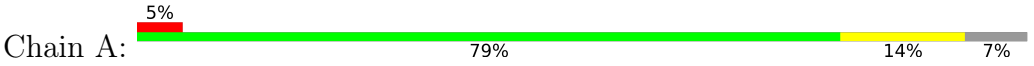
Chain	Residue	Modelled	Actual	Comment	Reference
C	474	HIS	-	expression tag	UNP A0A085R2T8
D	469	HIS	-	expression tag	UNP A0A085R2T8
D	470	HIS	-	expression tag	UNP A0A085R2T8
D	471	HIS	-	expression tag	UNP A0A085R2T8
D	472	HIS	-	expression tag	UNP A0A085R2T8
D	473	HIS	-	expression tag	UNP A0A085R2T8
D	474	HIS	-	expression tag	UNP A0A085R2T8
E	469	HIS	-	expression tag	UNP A0A085R2T8
E	470	HIS	-	expression tag	UNP A0A085R2T8
E	471	HIS	-	expression tag	UNP A0A085R2T8
E	472	HIS	-	expression tag	UNP A0A085R2T8
E	473	HIS	-	expression tag	UNP A0A085R2T8
E	474	HIS	-	expression tag	UNP A0A085R2T8
F	469	HIS	-	expression tag	UNP A0A085R2T8
F	470	HIS	-	expression tag	UNP A0A085R2T8
F	471	HIS	-	expression tag	UNP A0A085R2T8
F	472	HIS	-	expression tag	UNP A0A085R2T8
F	473	HIS	-	expression tag	UNP A0A085R2T8
F	474	HIS	-	expression tag	UNP A0A085R2T8

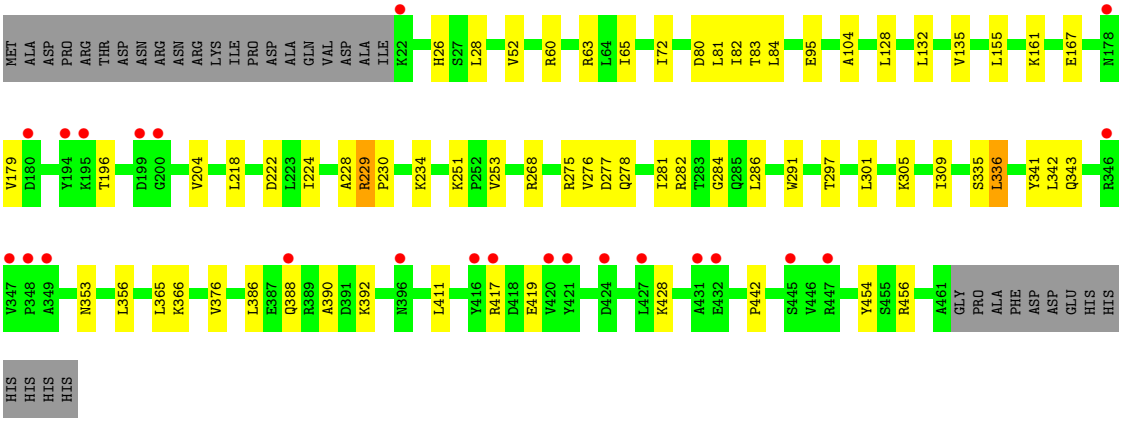
3 Residue-property plots (i)

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: Replicative DNA helicase

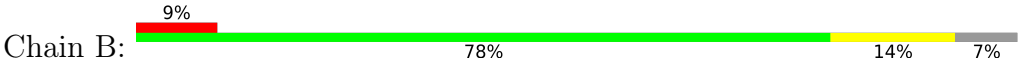
Chain A:

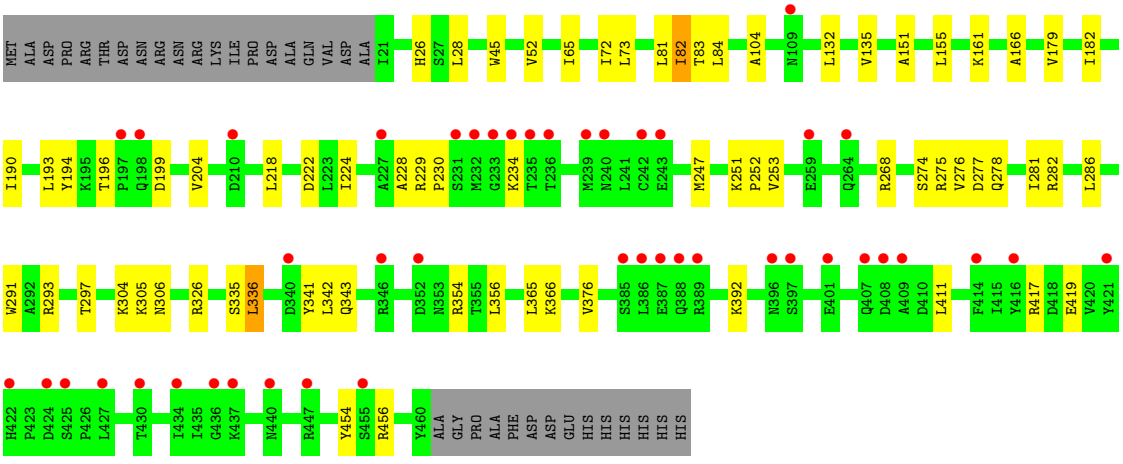




• Molecule 1: Replicative DNA helicase

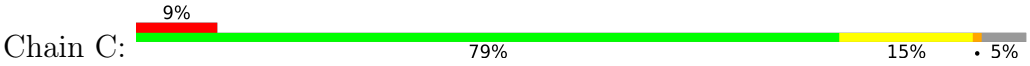
Chain B:

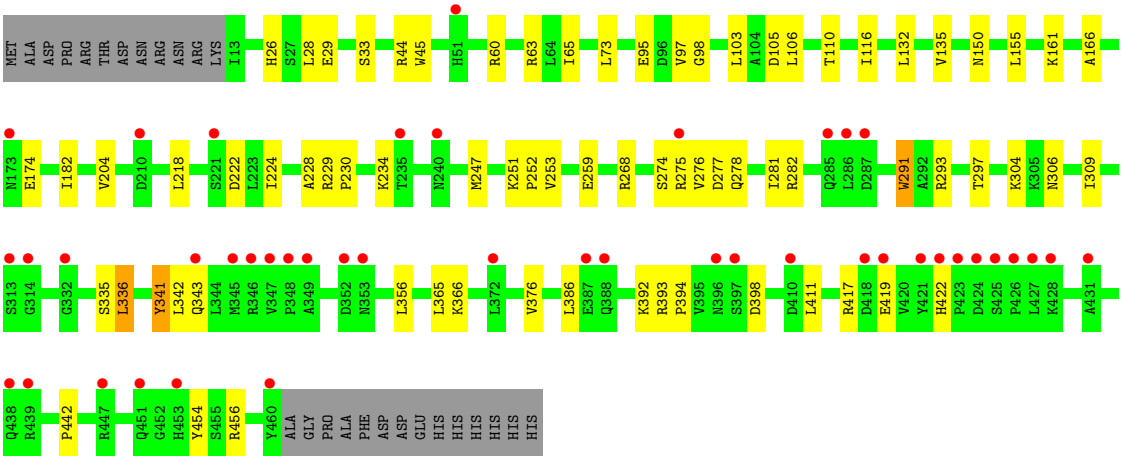




• Molecule 1: Replicative DNA helicase

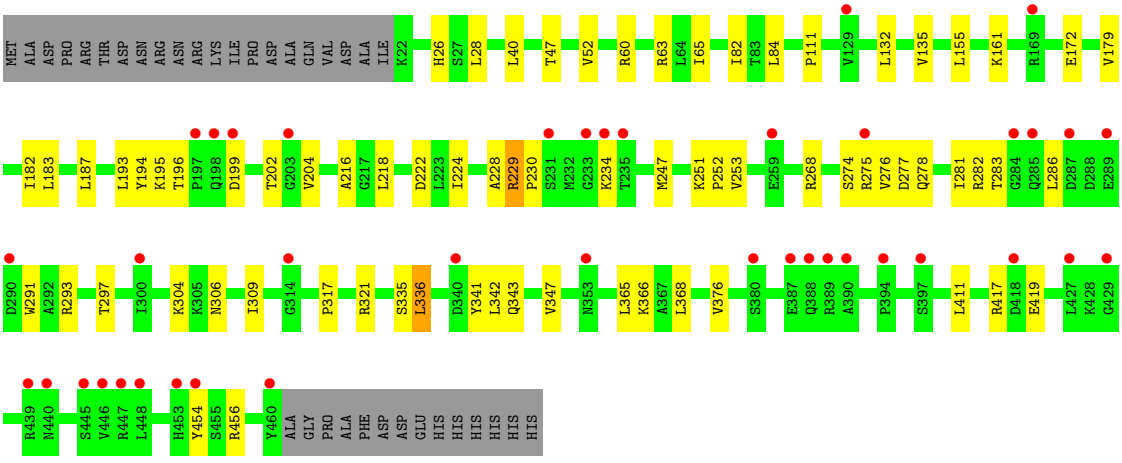
Chain C:





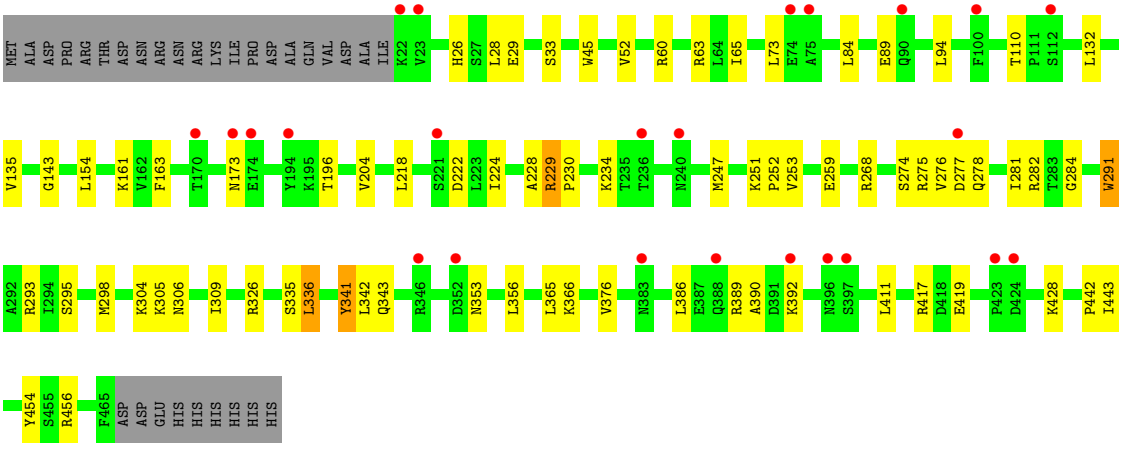
• Molecule 1: Replicative DNA helicase

Chain D:



• Molecule 1: Replicative DNA helicase

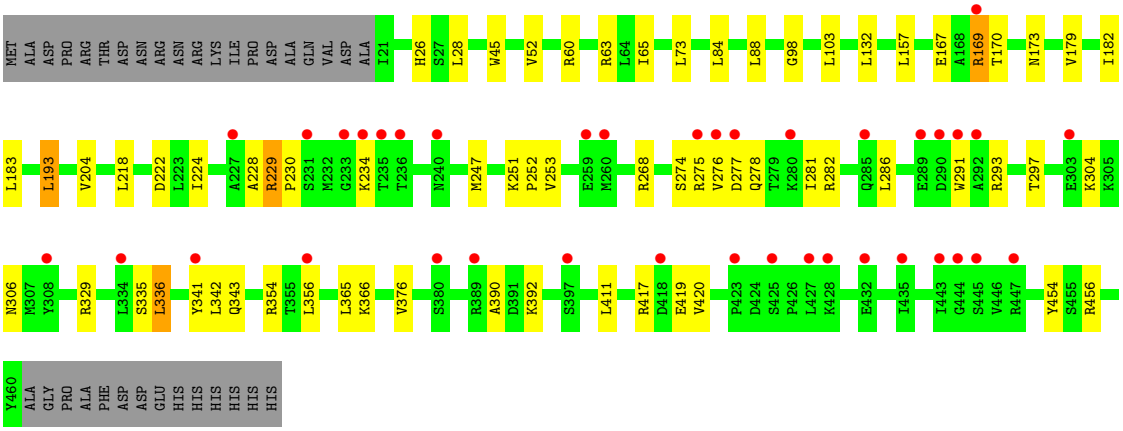
Chain E:



• Molecule 1: Replicative DNA helicase

Chain F:


8%
79%
13%
7%


MET ALA ASP PRO ARG THR ASP ASN ARG ASN ARG LYS ILE PRO ASP ALA GLN VAL ASP ALA I21 H26 S27 L28 W45 V52 R60 R63 L64 I65 L73 L84 L88 G98 L103 L132 L157 E167 A168 R169 T170 N173 V179 I182
L183 L193 V204 L218 D222 L223 I224 A227 A228 R229 P230 S231 M232 G233 K234 T235 T236 M240 M247 K251 P252 V253 E259 M260 R268 S274 R275 V276 D277 Q278 T279 K280 I281 R282 Q285 L286 E289 D290 W291 A292 R293 T297 E303 K304 K305
N306 M307 Y308 R329 L334 S335 L336 Y341 L342 Q343 R354 T355 L356 L365 K366 V376 S380 R389 A390 D391 K392 S397 L411 R417 D418 E419 V420 P423 D424 S425 P426 L427 K428 E432 I435 I443 G444 S445 V446 R447 Y454 S455 R456
Y460 ALA GLY PRO ALA PHE ASP ASP GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	141.23Å 150.10Å 188.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.63 – 3.80 32.63 – 3.80	Depositor EDS
% Data completeness (in resolution range)	72.7 (32.63-3.80) 72.7 (32.63-3.80)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.75Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.266 , 0.274 0.289 , 0.300	Depositor DCC
R_{free} test set	1408 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	152.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	20679	wwPDB-VP
Average B, all atoms (Å^2)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.19	0/3482	0.37	0/4708
1	B	0.19	0/3485	0.37	0/4712
1	C	0.20	0/3543	0.37	0/4793
1	D	0.20	0/3477	0.37	0/4701
1	E	0.20	0/3511	0.37	0/4748
1	F	0.20	0/3477	0.37	0/4701
All	All	0.19	0/20975	0.37	0/28363

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3433	0	3441	44	0
1	B	3436	0	3447	40	0
1	C	3493	0	3500	42	0
1	D	3428	0	3436	51	0
1	E	3460	0	3465	50	0
1	F	3429	0	3440	39	0
All	All	20679	0	20729	231	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (231) 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:F:60:ARG:HH11	1:F:63:ARG:HH12	1.10	0.99
1:D:60:ARG:HH11	1:D:63:ARG:HH12	1.11	0.99
1:A:60:ARG:HH11	1:A:63:ARG:HH12	1.12	0.96
1:E:60:ARG:HH11	1:E:63:ARG:HH12	1.11	0.94
1:C:60:ARG:HH11	1:C:63:ARG:HH12	1.10	0.93
1:F:60:ARG:HH11	1:F:63:ARG:NH1	1.73	0.87
1:A:60:ARG:HH11	1:A:63:ARG:NH1	1.73	0.87
1:D:60:ARG:HH11	1:D:63:ARG:NH1	1.73	0.86
1:E:60:ARG:HH11	1:E:63:ARG:NH1	1.74	0.86
1:C:60:ARG:HH11	1:C:63:ARG:NH1	1.74	0.85
1:C:60:ARG:NH1	1:C:63:ARG:HH12	1.77	0.83
1:E:60:ARG:NH1	1:E:63:ARG:HH12	1.78	0.82
1:F:60:ARG:NH1	1:F:63:ARG:HH12	1.76	0.81
1:D:60:ARG:NH1	1:D:63:ARG:HH12	1.78	0.81
1:A:60:ARG:NH1	1:A:63:ARG:HH12	1.79	0.80
1:A:390:ALA:HA	1:A:392:LYS:NZ	2.02	0.74
1:D:196:THR:HB	1:D:199:ASP:HB2	1.70	0.74
1:D:47:THR:HG22	1:E:326:ARG:HE	1.52	0.72
1:D:222:ASP:HA	1:D:366:LYS:NZ	2.06	0.70
1:B:222:ASP:HA	1:B:366:LYS:NZ	2.06	0.70
1:F:222:ASP:HA	1:F:366:LYS:NZ	2.06	0.69
1:A:222:ASP:HA	1:A:366:LYS:NZ	2.07	0.69
1:C:222:ASP:HA	1:C:366:LYS:NZ	2.07	0.69
1:E:222:ASP:HA	1:E:366:LYS:NZ	2.07	0.69
1:D:183:LEU:HD21	1:E:298:MET:HG3	1.75	0.68
1:D:286:LEU:HD11	1:D:291:TRP:CD1	2.29	0.68
1:A:390:ALA:HA	1:A:392:LYS:HZ3	1.59	0.67
1:D:82:ILE:HD11	1:E:29:GLU:HB2	1.79	0.65
1:E:26:HIS:CD2	1:E:28:LEU:HG	2.32	0.64
1:D:268:ARG:HH21	1:D:282:ARG:HH22	1.46	0.64
1:B:268:ARG:HH21	1:B:282:ARG:HH22	1.46	0.64
1:D:26:HIS:CD2	1:D:28:LEU:HG	2.32	0.64
1:B:26:HIS:CD2	1:B:28:LEU:HG	2.33	0.64
1:C:60:ARG:NH1	1:C:63:ARG:NH1	2.43	0.63
1:A:204:VAL:HB	1:A:218:LEU:HB2	1.81	0.63
1:A:268:ARG:HH21	1:A:282:ARG:HH22	1.47	0.63
1:B:204:VAL:HB	1:B:218:LEU:HB2	1.81	0.63
1:F:228:ALA:HB3	1:F:234:LYS:HB3	1.81	0.63
1:E:268:ARG:HH21	1:E:282:ARG:HH22	1.46	0.63
1:E:274:SER:HB3	1:E:293:ARG:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:VAL:HB	1:D:218:LEU:HB2	1.81	0.62
1:E:204:VAL:HB	1:E:218:LEU:HB2	1.81	0.62
1:B:82:ILE:HD11	1:C:29:GLU:HB2	1.80	0.62
1:A:26:HIS:CD2	1:A:28:LEU:HG	2.35	0.62
1:C:268:ARG:HH21	1:C:282:ARG:HH22	1.48	0.62
1:F:204:VAL:HB	1:F:218:LEU:HB2	1.81	0.62
1:C:204:VAL:HB	1:C:218:LEU:HB2	1.81	0.61
1:A:167:GLU:HG3	1:B:326:ARG:HD3	1.81	0.61
1:D:47:THR:CG2	1:E:326:ARG:HE	2.14	0.61
1:D:222:ASP:HA	1:D:366:LYS:HZ1	1.65	0.61
1:B:222:ASP:HA	1:B:366:LYS:HZ3	1.67	0.60
1:F:222:ASP:HA	1:F:366:LYS:HZ2	1.66	0.60
1:A:286:LEU:HD11	1:A:291:TRP:CD1	2.36	0.59
1:F:365:LEU:HD12	1:F:376:VAL:HG11	1.85	0.59
1:E:229:ARG:HG3	1:E:230:PRO:HD2	1.84	0.59
1:C:442:PRO:HB3	1:D:283:THR:HA	1.84	0.59
1:B:365:LEU:HD12	1:B:376:VAL:HG11	1.85	0.59
1:D:60:ARG:NH1	1:D:63:ARG:NH1	2.43	0.59
1:F:286:LEU:HD11	1:F:291:TRP:CD1	2.37	0.59
1:A:365:LEU:HD12	1:A:376:VAL:HG11	1.85	0.59
1:D:26:HIS:HD2	1:D:28:LEU:HG	1.67	0.58
1:D:229:ARG:HG3	1:D:230:PRO:HD2	1.86	0.58
1:D:365:LEU:HD12	1:D:376:VAL:HG11	1.85	0.58
1:F:60:ARG:NH1	1:F:63:ARG:NH1	2.42	0.58
1:E:365:LEU:HD12	1:E:376:VAL:HG11	1.84	0.58
1:F:229:ARG:HG3	1:F:230:PRO:HD2	1.86	0.58
1:A:26:HIS:HD2	1:A:28:LEU:HG	1.68	0.58
1:C:365:LEU:HD12	1:C:376:VAL:HG11	1.85	0.58
1:E:222:ASP:HA	1:E:366:LYS:HZ3	1.66	0.58
1:E:60:ARG:NH1	1:E:63:ARG:NH1	2.45	0.58
1:A:222:ASP:HA	1:A:366:LYS:HZ2	1.69	0.57
1:B:72:ILE:HD13	1:B:83:THR:HG22	1.87	0.57
1:B:26:HIS:HD2	1:B:28:LEU:HG	1.69	0.57
1:A:60:ARG:NH1	1:A:63:ARG:NH1	2.44	0.56
1:B:228:ALA:HB3	1:B:234:LYS:HB3	1.87	0.56
1:D:277:ASP:HA	1:D:454:TYR:HB3	1.88	0.56
1:E:277:ASP:HA	1:E:454:TYR:HB3	1.87	0.56
1:B:277:ASP:HA	1:B:454:TYR:HB3	1.88	0.56
1:F:277:ASP:HA	1:F:454:TYR:HB3	1.87	0.56
1:C:166:ALA:HB2	1:D:155:LEU:HD21	1.87	0.56
1:C:277:ASP:HA	1:C:454:TYR:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:ALA:HB3	1:E:234:LYS:HB3	1.87	0.56
1:E:26:HIS:HD2	1:E:28:LEU:HG	1.69	0.56
1:A:388:GLN:HB3	1:B:392:LYS:HZ1	1.72	0.55
1:A:277:ASP:HA	1:A:454:TYR:HB3	1.88	0.55
1:C:228:ALA:HB3	1:C:234:LYS:HB3	1.89	0.55
1:A:228:ALA:HB3	1:A:234:LYS:HB3	1.88	0.55
1:C:276:VAL:HG23	1:C:281:ILE:HD11	1.88	0.55
1:C:442:PRO:CB	1:D:283:THR:HA	2.37	0.54
1:D:276:VAL:HG23	1:D:281:ILE:HD11	1.89	0.54
1:C:33:SER:HA	1:C:110:THR:HG22	1.89	0.54
1:D:321:ARG:HG2	1:D:368:LEU:HD13	1.90	0.54
1:E:163:PHE:CZ	1:F:329:ARG:NH2	2.76	0.54
1:D:228:ALA:HB3	1:D:234:LYS:HB3	1.89	0.53
1:E:276:VAL:HG23	1:E:281:ILE:HD11	1.90	0.53
1:B:286:LEU:HD11	1:B:291:TRP:CD1	2.43	0.53
1:C:222:ASP:HA	1:C:366:LYS:HZ2	1.72	0.53
1:D:47:THR:HG22	1:E:326:ARG:NE	2.22	0.53
1:F:276:VAL:HG23	1:F:281:ILE:HD11	1.89	0.53
1:B:274:SER:HB3	1:B:293:ARG:HB3	1.89	0.53
1:A:276:VAL:HG23	1:A:281:ILE:HD11	1.89	0.53
1:D:274:SER:HB3	1:D:293:ARG:HB3	1.91	0.53
1:C:135:VAL:HG13	1:C:161:LYS:HB3	1.91	0.52
1:B:229:ARG:HG3	1:B:230:PRO:HD2	1.92	0.52
1:E:196:THR:HG21	1:E:442:PRO:HD3	1.90	0.52
1:A:253:VAL:HG12	1:A:336:LEU:HB3	1.92	0.52
1:C:44:ARG:HG3	1:C:116:ILE:HD13	1.90	0.52
1:C:222:ASP:HA	1:C:366:LYS:HZ3	1.74	0.51
1:D:252:PRO:HA	1:D:306:ASN:HB3	1.92	0.51
1:A:229:ARG:HG3	1:A:230:PRO:HD2	1.91	0.51
1:F:169:ARG:HD3	1:F:170:THR:HG23	1.90	0.51
1:D:253:VAL:HG12	1:D:336:LEU:HB3	1.93	0.51
1:E:143:GLY:HA2	1:E:154:LEU:HD21	1.91	0.51
1:E:252:PRO:HA	1:E:306:ASN:HB3	1.92	0.51
1:E:253:VAL:HG12	1:E:336:LEU:HB3	1.92	0.51
1:F:253:VAL:HG12	1:F:336:LEU:HB3	1.92	0.51
1:A:128:LEU:HB2	1:B:151:ALA:HB1	1.91	0.51
1:C:229:ARG:HG3	1:C:230:PRO:HD2	1.92	0.50
1:C:253:VAL:HG12	1:C:336:LEU:HB3	1.94	0.50
1:B:196:THR:HB	1:B:199:ASP:HB2	1.93	0.50
1:A:390:ALA:HA	1:A:392:LYS:HZ2	1.75	0.50
1:D:194:TYR:OH	1:E:291:TRP:NE1	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:TYR:CZ	1:E:291:TRP:NE1	2.77	0.50
1:B:253:VAL:HG12	1:B:336:LEU:HB3	1.92	0.50
1:F:390:ALA:HA	1:F:392:LYS:HE2	1.94	0.49
1:A:305:LYS:HA	1:F:179:VAL:HG21	1.93	0.49
1:E:353:ASN:HD21	1:F:354:ARG:HB2	1.77	0.49
1:F:252:PRO:HA	1:F:306:ASN:HB3	1.94	0.49
1:A:196:THR:HG21	1:A:442:PRO:HD3	1.93	0.49
1:C:274:SER:HB3	1:C:293:ARG:HB3	1.95	0.49
1:B:252:PRO:HA	1:B:306:ASN:HB3	1.94	0.48
1:F:274:SER:HB3	1:F:293:ARG:HB3	1.94	0.48
1:A:284:GLY:HA3	1:F:193:LEU:HB3	1.96	0.48
1:B:81:LEU:HD22	1:B:104:ALA:HA	1.95	0.48
1:C:247:MET:HA	1:C:304:LYS:HD3	1.95	0.48
1:C:392:LYS:NZ	1:C:422:HIS:NE2	2.55	0.48
1:B:65:ILE:HG23	1:B:84:LEU:HD21	1.95	0.48
1:E:247:MET:HA	1:E:304:LYS:HD3	1.95	0.48
1:A:286:LEU:CD1	1:A:291:TRP:CD1	2.96	0.48
1:B:247:MET:HA	1:B:304:LYS:HD3	1.97	0.47
1:B:45:TRP:HB2	1:B:73:LEU:HD13	1.96	0.47
1:B:190:ILE:HA	1:B:193:LEU:HD12	1.97	0.47
1:E:135:VAL:HG13	1:E:161:LYS:HB3	1.95	0.47
1:B:135:VAL:HG13	1:B:161:LYS:HB3	1.96	0.47
1:D:247:MET:HA	1:D:304:LYS:HD3	1.97	0.47
1:F:286:LEU:CD1	1:F:291:TRP:CD1	2.98	0.47
1:A:80:ASP:H	1:A:83:THR:HB	1.79	0.47
1:B:194:TYR:CZ	1:C:291:TRP:NE1	2.80	0.47
1:B:286:LEU:CD1	1:B:291:TRP:CD1	2.98	0.47
1:E:163:PHE:HZ	1:F:329:ARG:NH2	2.11	0.47
1:F:224:ILE:HG12	1:F:411:LEU:HD23	1.97	0.47
1:A:224:ILE:HG12	1:A:411:LEU:HD23	1.97	0.47
1:D:135:VAL:HG13	1:D:161:LYS:HB3	1.95	0.47
1:F:247:MET:HA	1:F:304:LYS:HD3	1.97	0.47
1:D:252:PRO:HB3	1:D:306:ASN:HA	1.97	0.47
1:A:309:ILE:HD12	1:F:182:ILE:HD13	1.97	0.46
1:D:286:LEU:CD1	1:D:291:TRP:CD1	2.96	0.46
1:E:224:ILE:HG12	1:E:411:LEU:HD23	1.97	0.46
1:C:224:ILE:HG12	1:C:411:LEU:HD23	1.97	0.46
1:D:317:PRO:HG2	1:D:347:VAL:HB	1.96	0.46
1:B:222:ASP:HA	1:B:366:LYS:HZ2	1.79	0.46
1:D:224:ILE:HG12	1:D:411:LEU:HD23	1.97	0.46
1:B:417:ARG:HG2	1:B:419:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:ARG:HG2	1:D:419:GLU:HG2	1.98	0.46
1:C:417:ARG:HG2	1:C:419:GLU:HG2	1.98	0.46
1:A:155:LEU:HD21	1:B:166:ALA:HB2	1.97	0.46
1:E:295:SER:HA	1:E:298:MET:HE2	1.98	0.45
1:A:179:VAL:HG21	1:B:305:LYS:HA	1.98	0.45
1:B:224:ILE:HG12	1:B:411:LEU:HD23	1.97	0.45
1:D:65:ILE:HG23	1:D:84:LEU:HD21	1.98	0.45
1:E:259:GLU:HB2	1:E:341:TYR:HD2	1.81	0.45
1:E:417:ARG:HG2	1:E:419:GLU:HG2	1.98	0.45
1:F:222:ASP:HA	1:F:366:LYS:HZ1	1.80	0.45
1:A:81:LEU:HD22	1:A:104:ALA:HA	1.99	0.45
1:A:275:ARG:HH21	1:A:456:ARG:NH1	2.15	0.45
1:B:276:VAL:HG23	1:B:281:ILE:HD11	1.97	0.45
1:A:417:ARG:HG2	1:A:419:GLU:HG2	1.98	0.45
1:D:187:LEU:HD21	1:E:298:MET:HE1	1.98	0.45
1:F:275:ARG:HH21	1:F:456:ARG:NH1	2.15	0.45
1:A:222:ASP:HA	1:A:366:LYS:HZ3	1.77	0.45
1:C:259:GLU:HB2	1:C:341:TYR:HD2	1.82	0.45
1:B:275:ARG:HH21	1:B:456:ARG:NH1	2.15	0.45
1:A:72:ILE:HD13	1:A:83:THR:HG22	1.99	0.45
1:A:132:LEU:HD11	1:B:155:LEU:HA	1.98	0.45
1:E:222:ASP:HA	1:E:366:LYS:HZ2	1.80	0.45
1:F:417:ARG:HG2	1:F:419:GLU:HG2	1.98	0.45
1:A:135:VAL:HG13	1:A:161:LYS:HB3	1.98	0.44
1:E:275:ARG:HH21	1:E:456:ARG:NH1	2.15	0.44
1:D:179:VAL:HG21	1:E:305:LYS:HA	1.98	0.44
1:A:301:LEU:HD23	1:F:183:LEU:HD11	1.98	0.44
1:D:193:LEU:HB3	1:E:284:GLY:HA3	1.98	0.44
1:E:390:ALA:HA	1:E:392:LYS:HE2	1.99	0.44
1:D:275:ARG:HH21	1:D:456:ARG:NH1	2.15	0.44
1:E:65:ILE:HG23	1:E:84:LEU:HD21	2.00	0.44
1:C:275:ARG:HH21	1:C:456:ARG:NH1	2.15	0.44
1:C:182:ILE:HG21	1:D:309:ILE:HD12	1.99	0.43
1:F:268:ARG:HH21	1:F:282:ARG:HH22	1.66	0.43
1:C:135:VAL:HG22	1:C:161:LYS:HD2	2.00	0.43
1:C:251:LYS:HB2	1:C:335:SER:HB3	2.01	0.43
1:D:202:THR:OG1	1:D:216:ALA:O	2.37	0.43
1:D:182:ILE:HD13	1:E:309:ILE:HD12	2.00	0.43
1:D:251:LYS:HB2	1:D:335:SER:HB3	2.01	0.43
1:F:26:HIS:CD2	1:F:28:LEU:HG	2.54	0.43
1:F:251:LYS:HB2	1:F:335:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:HIS:HD2	1:C:28:LEU:HG	1.83	0.42
1:A:353:ASN:HD21	1:B:354:ARG:HB2	1.84	0.42
1:B:182:ILE:HD13	1:C:309:ILE:HD12	2.00	0.42
1:A:251:LYS:HB2	1:A:335:SER:HB3	2.00	0.42
1:E:251:LYS:HB2	1:E:335:SER:HB3	2.01	0.42
1:E:389:ARG:O	1:F:420:VAL:O	2.37	0.42
1:B:194:TYR:CE2	1:C:291:TRP:NE1	2.82	0.42
1:F:88:LEU:HD12	1:F:103:LEU:HD11	2.01	0.42
1:B:251:LYS:HB2	1:B:335:SER:HB3	2.01	0.42
1:E:89:GLU:HB2	1:E:94:LEU:HD22	2.00	0.42
1:F:45:TRP:HB2	1:F:73:LEU:HD13	2.02	0.42
1:F:65:ILE:HG23	1:F:84:LEU:HD21	2.01	0.41
1:C:103:LEU:HA	1:C:106:LEU:HD12	2.02	0.41
1:C:252:PRO:HA	1:C:306:ASN:HB3	2.02	0.41
1:D:222:ASP:HA	1:D:366:LYS:HZ2	1.81	0.41
1:C:45:TRP:HB2	1:C:73:LEU:HD13	2.03	0.41
1:C:65:ILE:HD11	1:C:97:VAL:HG13	2.02	0.41
1:C:392:LYS:HZ3	1:C:422:HIS:CE1	2.37	0.40
1:C:393:ARG:HA	1:C:394:PRO:HD3	1.97	0.40
1:E:45:TRP:HB2	1:E:73:LEU:HD13	2.03	0.40
1:E:443:ILE:HD11	1:F:282:ARG:HD3	2.02	0.40
1:A:82:ILE:HD12	1:A:82:ILE:HA	1.96	0.40
1:D:286:LEU:HD11	1:D:291:TRP:CG	2.56	0.40
1:E:33:SER:HB3	1:E:110:THR:HG21	2.02	0.40
1:A:65:ILE:HG23	1:A:84:LEU:HD21	2.04	0.40
1:D:40:LEU:CD1	1:D:111:PRO:HA	2.52	0.40
1:D:196:THR:CB	1:D:199:ASP:HB2	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/474 (92%)	418 (95%)	20 (5%)	0	100	100
1	B	438/474 (92%)	413 (94%)	25 (6%)	0	100	100
1	C	446/474 (94%)	420 (94%)	25 (6%)	1 (0%)	47	79
1	D	437/474 (92%)	409 (94%)	27 (6%)	1 (0%)	47	79
1	E	442/474 (93%)	417 (94%)	25 (6%)	0	100	100
1	F	438/474 (92%)	410 (94%)	27 (6%)	1 (0%)	47	79
All	All	2639/2844 (93%)	2487 (94%)	149 (6%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	172	GLU
1	C	98	GLY
1	F	98	GLY

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	374/403 (93%)	362 (97%)	12 (3%)	39	65
1	B	375/403 (93%)	364 (97%)	11 (3%)	42	67
1	C	381/403 (94%)	365 (96%)	16 (4%)	30	58
1	D	374/403 (93%)	364 (97%)	10 (3%)	44	69
1	E	376/403 (93%)	363 (96%)	13 (4%)	36	64
1	F	374/403 (93%)	359 (96%)	15 (4%)	31	59
All	All	2254/2418 (93%)	2177 (97%)	77 (3%)	37	64

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	95	GLU

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Mol	Chain	Res	Type
1	A	229	ARG
1	A	278	GLN
1	A	297	THR
1	A	336	LEU
1	A	341	TYR
1	A	342	LEU
1	A	343	GLN
1	A	356	LEU
1	A	386	LEU
1	A	428	LYS
1	B	52	VAL
1	B	82	ILE
1	B	132	LEU
1	B	179	VAL
1	B	278	GLN
1	B	297	THR
1	B	336	LEU
1	B	341	TYR
1	B	342	LEU
1	B	343	GLN
1	B	356	LEU
1	C	95	GLU
1	C	105	ASP
1	C	132	LEU
1	C	150	ASN
1	C	155	LEU
1	C	174	GLU
1	C	278	GLN
1	C	291	TRP
1	C	297	THR
1	C	336	LEU
1	C	341	TYR
1	C	342	LEU
1	C	343	GLN
1	C	356	LEU
1	C	386	LEU
1	C	398	ASP
1	D	52	VAL
1	D	132	LEU
1	D	195	LYS
1	D	229	ARG
1	D	278	GLN

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Mol	Chain	Res	Type
1	D	297	THR
1	D	336	LEU
1	D	341	TYR
1	D	342	LEU
1	D	343	GLN
1	E	52	VAL
1	E	132	LEU
1	E	173	ASN
1	E	229	ARG
1	E	278	GLN
1	E	291	TRP
1	E	336	LEU
1	E	341	TYR
1	E	342	LEU
1	E	343	GLN
1	E	356	LEU
1	E	386	LEU
1	E	428	LYS
1	F	52	VAL
1	F	132	LEU
1	F	157	LEU
1	F	167	GLU
1	F	169	ARG
1	F	173	ASN
1	F	193	LEU
1	F	229	ARG
1	F	278	GLN
1	F	297	THR
1	F	336	LEU
1	F	341	TYR
1	F	342	LEU
1	F	343	GLN
1	F	356	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	407	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 monosaccharides 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	440/474 (92%)	0.38	23 (5%) 27 24	123, 171, 189, 194	0
1	B	440/474 (92%)	0.54	45 (10%) 6 6	116, 186, 228, 232	0
1	C	448/474 (94%)	0.61	44 (9%) 7 7	121, 194, 221, 230	0
1	D	439/474 (92%)	0.62	40 (9%) 9 7	120, 204, 246, 253	0
1	E	444/474 (93%)	0.40	24 (5%) 25 22	141, 168, 208, 219	0
1	F	440/474 (92%)	0.46	38 (8%) 10 8	125, 183, 205, 214	0
All	All	2651/2844 (93%)	0.50	214 (8%) 12 10	116, 179, 228, 253	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	GLY	6.9
1	B	198	GLN	6.5
1	F	444	GLY	6.0
1	B	421	TYR	5.9
1	B	396	ASN	5.8
1	B	236	THR	5.8
1	B	240	ASN	5.3
1	C	173	ASN	5.0
1	E	388	GLN	5.0
1	D	389	ARG	4.8
1	D	284	GLY	4.8
1	D	390	ALA	4.7
1	C	396	ASN	4.7
1	B	414	PHE	4.6
1	C	426	PRO	4.6
1	C	285	GLN	4.6
1	D	287	ASP	4.5
1	C	347	VAL	4.5
1	D	388	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	432	GLU	4.4
1	D	387	GLU	4.4
1	F	277	ASP	4.3
1	F	425	SER	4.3
1	D	290	ASP	4.3
1	C	345	MET	4.2
1	E	173	ASN	4.1
1	D	275	ARG	4.1
1	B	408	ASP	4.0
1	C	424	ASP	4.0
1	F	236	THR	3.9
1	A	178	ASN	3.9
1	C	418	ASP	3.9
1	D	259	GLU	3.8
1	D	427	LEU	3.8
1	F	445	SER	3.8
1	D	234	LYS	3.7
1	F	235	THR	3.7
1	B	197	PRO	3.7
1	D	233	GLY	3.6
1	F	233	GLY	3.6
1	C	313	SER	3.6
1	B	407	GLN	3.6
1	B	231	SER	3.6
1	C	410	ASP	3.5
1	C	431	ALA	3.5
1	D	285	GLN	3.5
1	D	235	THR	3.5
1	A	427	LEU	3.5
1	F	443	ILE	3.5
1	D	198	GLN	3.5
1	F	418	ASP	3.5
1	A	421	TYR	3.5
1	C	314	GLY	3.5
1	F	428	LYS	3.4
1	C	421	TYR	3.4
1	B	401	GLU	3.4
1	A	431	ALA	3.4
1	F	259	GLU	3.4
1	D	203	GLY	3.4
1	F	435	ILE	3.4
1	F	285	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	419	GLU	3.4
1	D	440	ASN	3.3
1	E	277	ASP	3.3
1	C	425	SER	3.3
1	A	388	GLN	3.3
1	C	235	THR	3.3
1	D	314	GLY	3.3
1	E	23	VAL	3.3
1	B	234	LYS	3.3
1	B	416	TYR	3.2
1	F	341	TYR	3.2
1	C	423	PRO	3.2
1	C	353	ASN	3.2
1	C	460	TYR	3.1
1	F	291	TRP	3.1
1	C	438	GLN	3.1
1	D	447	ARG	3.1
1	C	388	GLN	3.1
1	D	454	TYR	3.1
1	F	275	ARG	3.1
1	C	210	ASP	3.1
1	D	445	SER	3.1
1	B	235	THR	3.0
1	D	446	VAL	3.0
1	C	422	HIS	3.0
1	D	197	PRO	3.0
1	D	289	GLU	3.0
1	B	227	ALA	3.0
1	A	199	ASP	3.0
1	C	343	GLN	3.0
1	B	389	ARG	3.0
1	A	348	PRO	3.0
1	C	221	SER	2.9
1	B	259	GLU	2.9
1	E	22	LYS	2.9
1	E	240	ASN	2.9
1	A	424	ASP	2.9
1	E	236	THR	2.9
1	F	308	TYR	2.9
1	D	380	SER	2.9
1	E	174	GLU	2.9
1	D	439	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	75	ALA	2.9
1	C	287	ASP	2.8
1	A	447	ARG	2.8
1	B	109	ASN	2.8
1	F	231	SER	2.8
1	F	397	SER	2.8
1	B	232	MET	2.8
1	F	427	LEU	2.8
1	F	234	LYS	2.8
1	A	396	ASN	2.8
1	F	380	SER	2.8
1	B	264	GLN	2.7
1	B	388	GLN	2.7
1	B	434	ILE	2.7
1	B	447	ARG	2.7
1	C	397	SER	2.7
1	A	349	ALA	2.7
1	C	349	ALA	2.7
1	E	396	ASN	2.7
1	C	428	LYS	2.7
1	B	340	ASP	2.7
1	C	275	ARG	2.7
1	C	286	LEU	2.7
1	F	289	GLU	2.6
1	F	334	LEU	2.6
1	B	436	GLY	2.6
1	B	242	CYS	2.6
1	B	385	SER	2.6
1	A	180	ASP	2.5
1	D	231	SER	2.5
1	C	346	ARG	2.5
1	D	129	VAL	2.5
1	D	353	ASN	2.5
1	B	424	ASP	2.4
1	E	383	ASN	2.4
1	A	346	ARG	2.4
1	A	195	LYS	2.4
1	C	451	GLN	2.4
1	E	194	TYR	2.4
1	B	243	GLU	2.4
1	E	112	SER	2.4
1	E	397	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	427	LEU	2.4
1	D	199	ASP	2.4
1	D	300	ILE	2.4
1	D	418	ASP	2.4
1	C	240	ASN	2.3
1	C	387	GLU	2.3
1	F	447	ARG	2.3
1	B	386	LEU	2.3
1	F	356	LEU	2.3
1	C	352	ASP	2.3
1	A	22	LYS	2.3
1	D	448	LEU	2.3
1	D	169	ARG	2.3
1	A	417	ARG	2.3
1	C	51	HIS	2.3
1	E	423	PRO	2.3
1	C	332	GLY	2.3
1	D	429	GLY	2.3
1	D	397	SER	2.3
1	A	420	VAL	2.3
1	F	276	VAL	2.3
1	B	409	ALA	2.2
1	B	422	HIS	2.2
1	C	372	LEU	2.2
1	D	453	HIS	2.2
1	A	347	VAL	2.2
1	B	239	MET	2.2
1	A	445	SER	2.2
1	E	221	SER	2.2
1	F	423	PRO	2.2
1	F	292	ALA	2.2
1	A	200	GLY	2.2
1	F	169	ARG	2.2
1	C	453	HIS	2.2
1	F	227	ALA	2.2
1	A	194	TYR	2.2
1	C	447	ARG	2.2
1	D	394	PRO	2.2
1	F	303	GLU	2.2
1	B	210	ASP	2.2
1	D	460	TYR	2.2
1	E	346	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	100	PHE	2.1
1	C	348	PRO	2.1
1	B	427	LEU	2.1
1	B	346	ARG	2.1
1	B	430	THR	2.1
1	F	389	ARG	2.1
1	F	280	LYS	2.1
1	F	260	MET	2.1
1	E	392	LYS	2.1
1	B	397	SER	2.1
1	E	424	ASP	2.1
1	D	340	ASP	2.1
1	F	432	GLU	2.1
1	E	90	GLN	2.1
1	B	425	SER	2.1
1	F	290	ASP	2.1
1	F	240	ASN	2.1
1	E	170	THR	2.0
1	B	440	ASN	2.0
1	B	387	GLU	2.0
1	C	439	ARG	2.0
1	B	455	SER	2.0
1	B	352	ASP	2.0
1	B	437	LYS	2.0
1	E	74	GLU	2.0
1	E	352	ASP	2.0
1	A	416	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.