wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 09:14 AM EDT

PDB ID	:	3UPU
Title	:	Crystal structure of the T4 Phage SF1B Helicase Dda
Authors	:	He, X.; Yun, M.K.; Pemble IV, C.W.; Kreuzer, K.N.; Raney, K.D.; White, S.W.
Deposited on	:	2011-11-18
Resolution	:	3.30 Å(reported)

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

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

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

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

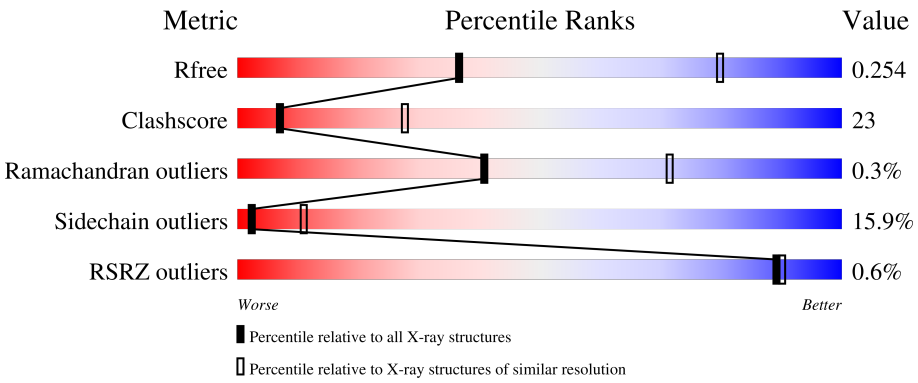
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	459	48% 39% 8% •
1	B	459	47% 41% 8% •
1	C	459	% 50% 38% 8% •
2	D	8	25% 75%
2	E	8	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	8	12% 50% 50%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11054 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 ATP-dependent DNA helicase dda.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	439	3529	2280	582	655	5	7	0	1	0
1	B	439	3522	2275	580	655	5	7	0	0	0
1	C	439	3522	2275	580	655	5	7	0	0	0

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP P32270
A	-18	GLY	-	EXPRESSION TAG	UNP P32270
A	-17	SER	-	EXPRESSION TAG	UNP P32270
A	-16	SER	-	EXPRESSION TAG	UNP P32270
A	-15	HIS	-	EXPRESSION TAG	UNP P32270
A	-14	HIS	-	EXPRESSION TAG	UNP P32270
A	-13	HIS	-	EXPRESSION TAG	UNP P32270
A	-12	HIS	-	EXPRESSION TAG	UNP P32270
A	-11	HIS	-	EXPRESSION TAG	UNP P32270
A	-10	HIS	-	EXPRESSION TAG	UNP P32270
A	-9	SER	-	EXPRESSION TAG	UNP P32270
A	-8	SER	-	EXPRESSION TAG	UNP P32270
A	-7	GLY	-	EXPRESSION TAG	UNP P32270
A	-6	LEU	-	EXPRESSION TAG	UNP P32270
A	-5	VAL	-	EXPRESSION TAG	UNP P32270
A	-4	PRO	-	EXPRESSION TAG	UNP P32270
A	-3	ARG	-	EXPRESSION TAG	UNP P32270
A	-2	GLY	-	EXPRESSION TAG	UNP P32270
A	-1	SER	-	EXPRESSION TAG	UNP P32270
A	0	HIS	-	EXPRESSION TAG	UNP P32270
A	38	ALA	LYS	ENGINEERED MUTATION	UNP P32270
A	54	GLU	GLY	SEE REMARK 999	UNP P32270
A	151	ASP	GLU	SEE REMARK 999	UNP P32270

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Chain	Residue	Modelled	Actual	Comment	Reference
A	196	ILE	ASN	SEE REMARK 999	UNP P32270
A	357	GLY	ALA	SEE REMARK 999	UNP P32270
B	-19	MSE	-	EXPRESSION TAG	UNP P32270
B	-18	GLY	-	EXPRESSION TAG	UNP P32270
B	-17	SER	-	EXPRESSION TAG	UNP P32270
B	-16	SER	-	EXPRESSION TAG	UNP P32270
B	-15	HIS	-	EXPRESSION TAG	UNP P32270
B	-14	HIS	-	EXPRESSION TAG	UNP P32270
B	-13	HIS	-	EXPRESSION TAG	UNP P32270
B	-12	HIS	-	EXPRESSION TAG	UNP P32270
B	-11	HIS	-	EXPRESSION TAG	UNP P32270
B	-10	HIS	-	EXPRESSION TAG	UNP P32270
B	-9	SER	-	EXPRESSION TAG	UNP P32270
B	-8	SER	-	EXPRESSION TAG	UNP P32270
B	-7	GLY	-	EXPRESSION TAG	UNP P32270
B	-6	LEU	-	EXPRESSION TAG	UNP P32270
B	-5	VAL	-	EXPRESSION TAG	UNP P32270
B	-4	PRO	-	EXPRESSION TAG	UNP P32270
B	-3	ARG	-	EXPRESSION TAG	UNP P32270
B	-2	GLY	-	EXPRESSION TAG	UNP P32270
B	-1	SER	-	EXPRESSION TAG	UNP P32270
B	0	HIS	-	EXPRESSION TAG	UNP P32270
B	38	ALA	LYS	ENGINEERED MUTATION	UNP P32270
B	54	GLU	GLY	SEE REMARK 999	UNP P32270
B	151	ASP	GLU	SEE REMARK 999	UNP P32270
B	196	ILE	ASN	SEE REMARK 999	UNP P32270
B	357	GLY	ALA	SEE REMARK 999	UNP P32270
C	-19	MSE	-	EXPRESSION TAG	UNP P32270
C	-18	GLY	-	EXPRESSION TAG	UNP P32270
C	-17	SER	-	EXPRESSION TAG	UNP P32270
C	-16	SER	-	EXPRESSION TAG	UNP P32270
C	-15	HIS	-	EXPRESSION TAG	UNP P32270
C	-14	HIS	-	EXPRESSION TAG	UNP P32270
C	-13	HIS	-	EXPRESSION TAG	UNP P32270
C	-12	HIS	-	EXPRESSION TAG	UNP P32270
C	-11	HIS	-	EXPRESSION TAG	UNP P32270
C	-10	HIS	-	EXPRESSION TAG	UNP P32270
C	-9	SER	-	EXPRESSION TAG	UNP P32270
C	-8	SER	-	EXPRESSION TAG	UNP P32270
C	-7	GLY	-	EXPRESSION TAG	UNP P32270
C	-6	LEU	-	EXPRESSION TAG	UNP P32270
C	-5	VAL	-	EXPRESSION TAG	UNP P32270

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	EXPRESSION TAG	UNP P32270
C	-3	ARG	-	EXPRESSION TAG	UNP P32270
C	-2	GLY	-	EXPRESSION TAG	UNP P32270
C	-1	SER	-	EXPRESSION TAG	UNP P32270
C	0	HIS	-	EXPRESSION TAG	UNP P32270
C	38	ALA	LYS	ENGINEERED MUTATION	UNP P32270
C	54	GLU	GLY	SEE REMARK 999	UNP P32270
C	151	ASP	GLU	SEE REMARK 999	UNP P32270
C	196	ILE	ASN	SEE REMARK 999	UNP P32270
C	357	GLY	ALA	SEE REMARK 999	UNP P32270

- Molecule 2 is a DNA chain called 5'-D(*TP*TP*TP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	8	157	80	16	54	7	0	0	0
2	E	8	157	80	16	54	7	0	0	0
2	F	8	157	80	16	54	7	0	0	0

- Molecule 3 is water.

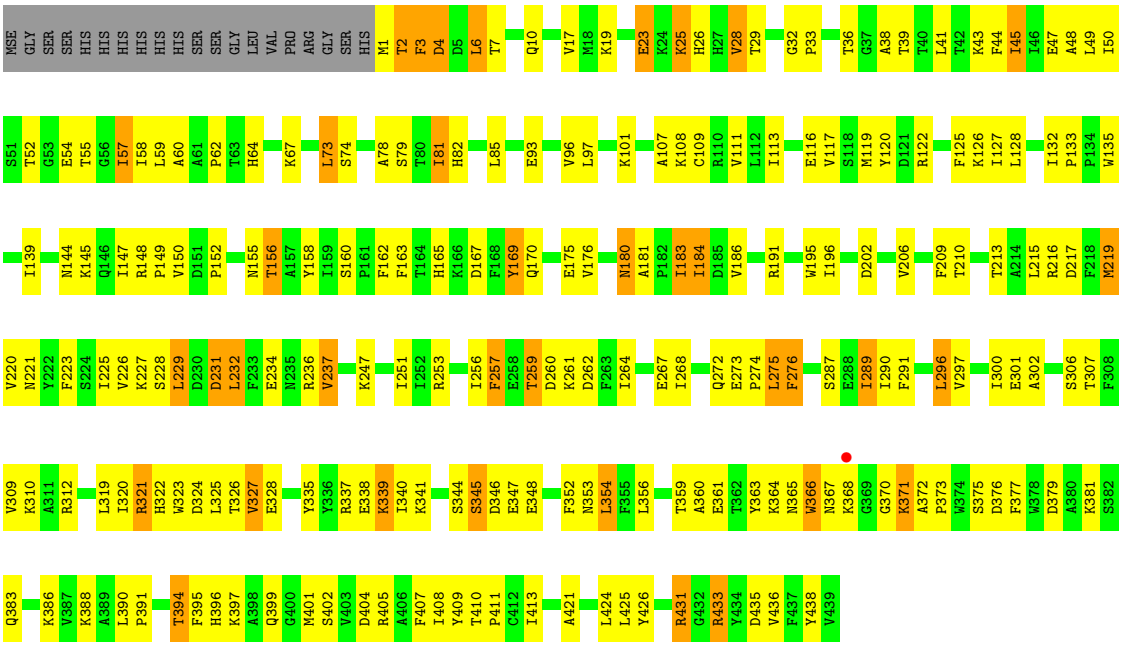
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	4	4	4	0	0
3	B	2	2	2	0	0
3	D	2	2	2	0	0
3	E	1	1	1	0	0
3	F	1	1	1	0	0

3 Residue-property plots (i)

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

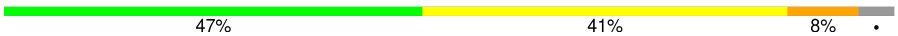
• Molecule 1: ATP-dependent DNA helicase dda

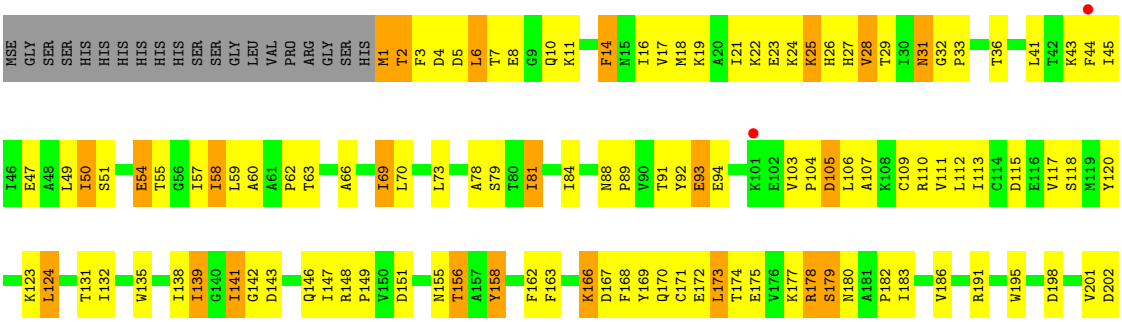
Chain A:



• Molecule 1: ATP-dependent DNA helicase dda

Chain B:





T210 G211 D212 T213 R216 D217 F218 M219 V220 N221 Y222 F223 S224 I225 V226 K227 S228 L229 D230 D231 L232 F233 E234 N235 R236 V237 I252 I256 F257 E258 T259 D260 K261 I268 M271 Q272 L275 F276 K277 T278 I281 K284 S287 E288 I289 I290 F291 Q295 L296

V297 I300 T305 S306 T307 F308 V309 K310 A311 V314 L319 I320 R321 H322 W323 D324 L325 T326 V327 E328 E334 R337 E338 K339 I340 K341 I342 I343 S344 S345 E348 L354 F355 T359 K364 N365 W366 N367 K371 A372 P373 Q383 F384 V387 K388 A389 L390

P391 F395 H396 K397 A398 Q399 G400 M401 S402 V403 D404 R405 A406 F407 I408 Y409 T410 P411 C412 I413 H414 Y415 A416 D417 V418 E419 L420 A421 Q422 Q423 L424 L425 Y426 V427 T430 R431 V436 V439

- Molecule 1: ATP-dependent DNA helicase dda

Chain C: % 50% 38% 8%

MSE GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS M1 T2 F3 D4 D5 L6 T7 Q10 K11 N12 A13 I16 V17 A20 K25 H26 H27 V28 T29 I30 N31 G32 G35 T36 G37 A38 T39 T40 L41 T42 K43 F44 I45 I46 E47

A48 L49 I50 E54 T55 G56 I57 I58 L59 A60 A61 P62 K67 L70 S71 K72 L73 K76 E77 A78 S79 T80 I81 H82 L85 E93 E94 N95 V96 L97 F98 K101 D105 L106 A107 K108 C109 R110 V111 L112 I113 C114 D115 E116 V117 S118 R122 K123 L124 F125 K126

I127 L128 I132 P133 C136 T137 I138 I139 G140 I141 K145 Q146 I147 R148 P149 V150 D151 E154 N155 T156 A157 Y158 I159 S160 P161 F162 F163 T164 H165 K166 D167 F168 Y169 Q170 C171 V176 K177 R178 S179 N180 A181 P182 I183 I184 D185 V186 V190 R191 K194 W195 K199 V200

V201 D202 F209 T213 R216 D217 V220 N221 Y222 F223 S224 I225 V226 K227 D231 L232 N235 R236 V237 T241 S244 V245 D246 K247 L248 I251 I252 I256 F257 E258 T259 D260 K261 I264 E267 Q272 E273 P274 L275 F276 K280 I281 I289 I290 F291

N292 Q295 L296 V297 I300 Y304 T305 S306 T307 K310 A311 R312 G313 V314 P315 L319 I320 R321 H322 W323 D324 L325 T326 V327 R337 E338 K339 I340 K341 I342 E348 L349 L354 F355 K358 T359 T362 N365 W366 N367 K368 K371 A372 P373 W374 S375 D376

D379 K388 A389 L390 P391 T394 F395 H396 S402 Y409 T410 P411 C412 I413 V418 E419 L420 A421 Q422 Q423 L424 L425 Y426 V427 T430 R431 V439

- Molecule 2: 5'-D(*TP*TP*TP*TP*TP*TP*TP*T)-3'

Chain D: 25% 75%

T600 T601 T602 T603 T604 T605 T606 T607

- Molecule 2: 5'-D(*TP*TP*TP*TP*TP*TP*TP*T)-3'

Chain E: 50% 50%

T600 T601 T602 T603 T604 T605 T606 T607

- Molecule 2: 5'-D(*TP*TP*TP*TP*TP*TP*TP*T)-3'

Chain F: 12% 50% 50%

T600
T601
T602
T603
T604
T605
T606
T607

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	225.54Å 107.25Å 85.47Å 90.00° 94.13° 90.00°	Depositor
Resolution (Å)	32.27 – 3.30 36.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	91.1 (32.27-3.30) 90.8 (36.04-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.204 , 0.258 0.201 , 0.254	Depositor DCC
R_{free} test set	1466 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	92.4	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 64.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11054	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.28	0/3607	0.51	0/4869
1	B	0.26	0/3596	0.47	0/4854
1	C	0.25	0/3596	0.47	0/4854
2	D	0.51	0/172	1.48	0/264
2	E	0.50	0/172	1.42	0/264
2	F	0.52	0/172	1.39	0/264
All	All	0.28	0/11315	0.57	0/15369

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	4
1	C	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	THR	Peptide
1	A	344	SER	Peptide
1	A	366	TRP	Peptide
1	A	4	ASP	Peptide
1	C	108	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3529	0	3549	175	0
1	B	3522	0	3542	163	0
1	C	3522	0	3542	156	0
2	D	157	0	98	8	0
2	E	157	0	98	5	0
2	F	157	0	98	9	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	11054	0	10927	504	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 23.

The worst 5 of 504 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:6:LEU:HD12	1:B:11:LYS:HG2	1.31	1.07
1:B:276:PHE:HE1	1:B:289:ILE:HG12	1.18	1.04
1:B:321:ARG:HG3	1:B:321:ARG:HH11	1.22	1.00
1:A:232:LEU:H	1:A:232:LEU:HD22	1.26	0.95
1:B:276:PHE:CE1	1:B:289:ILE:HG12	2.05	0.92

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	438/459 (95%)	408 (93%)	29 (7%)	1 (0%)	47	77
1	B	437/459 (95%)	397 (91%)	39 (9%)	1 (0%)	47	77
1	C	437/459 (95%)	402 (92%)	33 (8%)	2 (0%)	29	61
All	All	1312/1377 (95%)	1207 (92%)	101 (8%)	4 (0%)	41	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	93	GLU
1	C	93	GLU
1	A	93	GLU
1	C	256	ILE

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	386/394 (98%)	330 (86%)	56 (14%)	3	14
1	B	385/394 (98%)	316 (82%)	69 (18%)	2	8
1	C	385/394 (98%)	326 (85%)	59 (15%)	2	12
All	All	1156/1182 (98%)	972 (84%)	184 (16%)	2	11

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	348	GLU
1	C	118	SER
1	B	367	ASN
1	C	28	VAL
1	C	166	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	95	ASN
1	C	272	GLN
1	C	353	ASN
1	C	295	GLN
1	B	82	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	432/459 (94%)	-0.09	1 (0%) 95 96	62, 98, 136, 169	0
1	B	432/459 (94%)	-0.04	2 (0%) 91 91	64, 106, 159, 184	0
1	C	432/459 (94%)	0.03	4 (0%) 84 84	81, 115, 154, 180	0
2	D	8/8 (100%)	0.05	0 100 100	86, 91, 111, 160	0
2	E	8/8 (100%)	0.11	0 100 100	95, 104, 149, 197	0
2	F	8/8 (100%)	0.64	1 (12%) 3 3	106, 112, 161, 217	0
All	All	1320/1401 (94%)	-0.03	8 (0%) 89 90	62, 107, 155, 217	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	600	DT	5.1
1	C	180	ASN	3.5
1	C	371	LYS	3.0
1	C	202	ASP	2.6
1	C	178	ARG	2.4

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.