Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2025 – 04:39 PM EDT

PDB ID	:	9MRU / pdb_00009mru
Title	:	Structural Asymmetry in SARS-CoV-2 Nsp15 Hexamer Important for Catalytic Activity
Authors	:	Ketawala, G.K.; Sonowal, M.; Schrag, L.; Fromme, R.; Botha, S.; Fromme, P.
Deposited on	:	2025-01-08
Resolution	:	3.00 Å(reported)

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

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

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

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

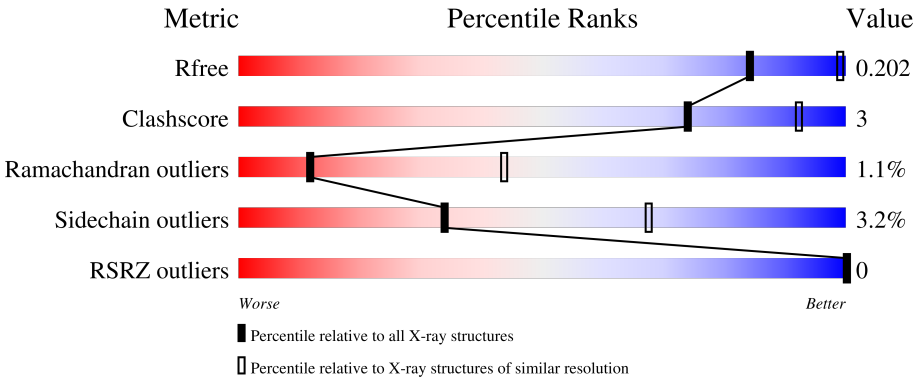
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	347	88% 11% •
1	B	347	90% 9% •
1	C	347	91% 8% •
1	D	347	86% 12% •
1	E	347	87% 12% •

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Mol	Chain	Length	Quality of chain
1	F	347	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16476 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 Uridylate-specific endoribonuclease nsp15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2746	1765	448	522	11			
1	B	347	Total	C	N	O	S	0	0	0
			2746	1765	448	522	11			
1	C	347	Total	C	N	O	S	0	0	0
			2746	1765	448	522	11			
1	D	347	Total	C	N	O	S	0	0	0
			2746	1765	448	522	11			
1	E	347	Total	C	N	O	S	0	0	0
			2746	1765	448	522	11			
1	F	347	Total	C	N	O	S	0	0	0
			2746	1765	448	522	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P0DTD1
A	1	MET	-	expression tag	UNP P0DTD1
A	267	GLN	GLU	engineered mutation	UNP P0DTD1
B	0	HIS	-	expression tag	UNP P0DTD1
B	1	MET	-	expression tag	UNP P0DTD1
B	267	GLN	GLU	engineered mutation	UNP P0DTD1
C	0	HIS	-	expression tag	UNP P0DTD1
C	1	MET	-	expression tag	UNP P0DTD1
C	267	GLN	GLU	engineered mutation	UNP P0DTD1
D	0	HIS	-	expression tag	UNP P0DTD1
D	1	MET	-	expression tag	UNP P0DTD1
D	267	GLN	GLU	engineered mutation	UNP P0DTD1
E	0	HIS	-	expression tag	UNP P0DTD1
E	1	MET	-	expression tag	UNP P0DTD1
E	267	GLN	GLU	engineered mutation	UNP P0DTD1
F	0	HIS	-	expression tag	UNP P0DTD1
F	1	MET	-	expression tag	UNP P0DTD1

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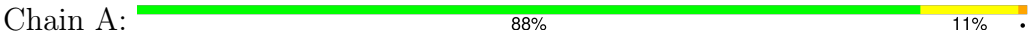
Chain	Residue	Modelled	Actual	Comment	Reference
F	267	GLN	GLU	engineered mutation	UNP P0DTD1

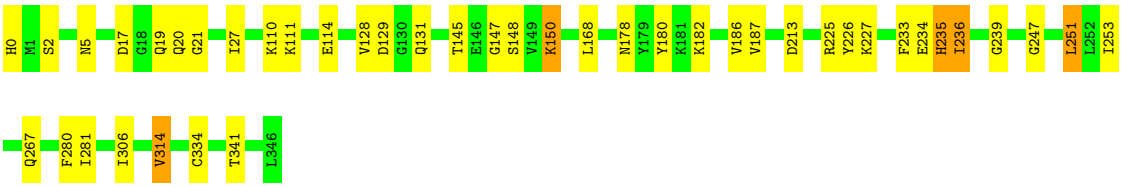
3 Residue-property plots (i)

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: Uridylate-specific endoribonuclease nsp15

Chain A:





• Molecule 1: Uridylate-specific endoribonuclease nsp15

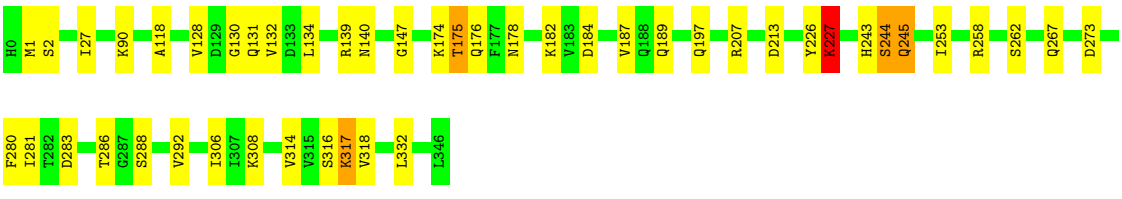
Chain B:

• Molecule 1: Uridylate-specific endoribonuclease nsp15

Chain C:

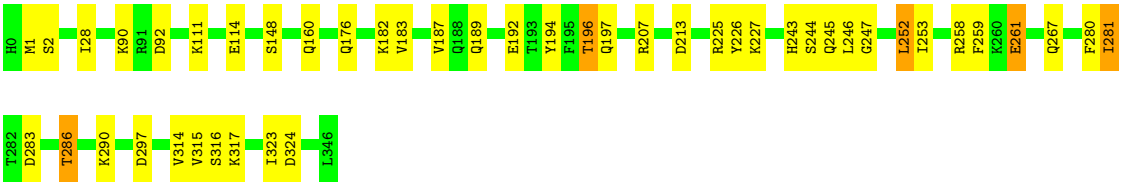
• Molecule 1: Uridylate-specific endoribonuclease nsp15

Chain D:



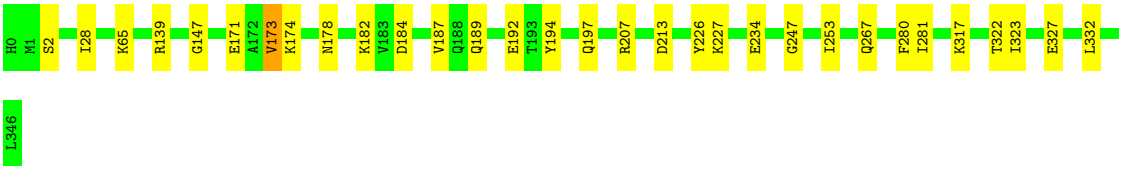
• Molecule 1: Uridylate-specific endoribonuclease nsp15

Chain E:



• Molecule 1: Uridylate-specific endoribonuclease nsp15

Chain F:



4 Data and refinement statistics (i)

Property	Value	Sourc
Space group	P 1 21 1	Deposi
Cell constants a, b, c, α, β, γ	154.70Å 116.60Å 154.80Å 90.00° 119.40° 90.00°	Deposi
Resolution (Å)	29.98 – 3.00 29.98 – 3.00	Deposi EDS
% Data completeness (in resolution range)	100.0 (29.98-3.00) 96.8 (29.98-3.00)	Deposi EDS
R_{merge}	(Not available)	Deposi
R_{sym}	(Not available)	Deposi
$< I/\sigma(I) >$ [1]	1.10 (at 3.00Å)	Xtriag
Refinement program	PHENIX (1.21.1_5286), REFMAC CCP4-V9.0, PDB-REDO	Deposi
R, R_{free}	0.185 , 0.211 0.180 , 0.202	Deposi DCC
R_{free} test set	4632 reflections (4.82%)	wwPDB
Wilson B-factor (Å^2)	86.0	Xtriag
Anisotropy	0.145	Xtriag
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriag
Estimated twinning fraction	0.357 for -h-l,k,h 0.357 for l,k,-h-l 0.357 for h,-k,-h-l 0.357 for -h-l,-k,l 0.378 for l,-k,h	Xtriag
F_o,F_c correlation	0.97	EDS
Total number of atoms	16476	wwPDB
Average B, all atoms (Å^2)	76.0	wwPDB

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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	0.08	0/2804	0.28	0/3802
1	B	0.08	0/2804	0.26	0/3802
1	C	0.08	0/2804	0.24	0/3802
1	D	0.09	0/2804	0.27	0/3802
1	E	0.11	0/2804	0.27	0/3802
1	F	0.08	0/2804	0.26	0/3802
All	All	0.09	0/16824	0.26	0/22812

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	2746	0	2741	21	0
1	B	2746	0	2741	18	0
1	C	2746	0	2741	12	0
1	D	2746	0	2741	21	0
1	E	2746	0	2741	19	0
1	F	2746	0	2741	14	0
All	All	16476	0	16446	99	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 3.

All (99) 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:267:GLN:HB2	1:F:280:PHE:HB3	1.72	0.71
1:E:281:ILE:HD11	1:E:290:LYS:HB3	1.73	0.70
1:D:243:HIS:O	1:D:245:GLN:N	2.24	0.67
1:E:194:TYR:HB2	1:E:323:ILE:HG13	1.77	0.67
1:D:317:LYS:NZ	1:D:332:LEU:O	2.29	0.65
1:E:243:HIS:O	1:E:245:GLN:N	2.27	0.63
1:D:130:GLY:O	1:D:132:VAL:N	2.30	0.62
1:B:268:ASP:O	1:B:270:ILE:N	2.32	0.61
1:E:267:GLN:HB2	1:E:280:PHE:HB3	1.83	0.60
1:B:258:ARG:NE	1:B:262:SER:OG	2.36	0.59
1:D:258:ARG:HE	1:D:262:SER:HB3	1.68	0.58
1:A:235:HIS:HA	1:A:239:GLY:H	1.69	0.58
1:B:268:ASP:C	1:B:270:ILE:H	2.13	0.57
1:A:17:ASP:OD2	1:A:19:GLN:NE2	2.30	0.57
1:E:314:VAL:HG21	1:E:317:LYS:HG3	1.87	0.57
1:A:182:LYS:HG2	1:A:187:VAL:HG22	1.86	0.57
1:D:213:ASP:OD2	1:D:226:TYR:OH	2.21	0.57
1:B:267:GLN:HB2	1:B:280:PHE:HB3	1.87	0.55
1:E:258:ARG:NH2	1:E:283:ASP:OD2	2.39	0.55
1:E:182:LYS:HG2	1:E:187:VAL:HG22	1.88	0.55
1:B:1:MET:N	1:B:1:MET:SD	2.79	0.55
1:D:147:GLY:O	1:D:178:ASN:ND2	2.39	0.54
1:A:267:GLN:HB2	1:A:280:PHE:HB3	1.88	0.54
1:C:182:LYS:HG2	1:C:187:VAL:HG22	1.88	0.54
1:D:267:GLN:HB2	1:D:280:PHE:HB3	1.90	0.54
1:E:196:THR:OG1	1:E:324:ASP:OD2	2.27	0.53
1:B:251:LEU:O	1:B:253:ILE:N	2.37	0.53
1:A:2:SER:HB2	1:D:2:SER:HB2	1.91	0.52
1:A:225:ARG:C	1:A:227:LYS:H	2.18	0.52
1:A:213:ASP:OD2	1:A:226:TYR:OH	2.28	0.52
1:A:235:HIS:O	1:A:236:ILE:HB	2.09	0.51
1:B:213:ASP:OD2	1:B:226:TYR:OH	2.28	0.51
1:C:213:ASP:OD2	1:C:226:TYR:OH	2.29	0.51
1:F:182:LYS:HG2	1:F:187:VAL:HG22	1.93	0.51
1:A:251:LEU:O	1:A:253:ILE:N	2.41	0.50
1:E:252:LEU:HD12	1:E:297:ASP:HB2	1.93	0.50
1:C:217:LEU:HB3	1:C:221:GLU:OE2	2.11	0.50
1:E:213:ASP:OD2	1:E:226:TYR:OH	2.26	0.50
1:E:281:ILE:H	1:E:281:ILE:HD13	1.77	0.50
1:A:168:LEU:HD23	1:C:284:ALA:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PHE:CD1	1:B:270:ILE:HG13	2.47	0.50
1:F:197:GLN:OE1	1:F:207:ARG:NH1	2.45	0.49
1:B:225:ARG:C	1:B:227:LYS:H	2.20	0.49
1:E:225:ARG:C	1:E:227:LYS:H	2.21	0.48
1:F:147:GLY:O	1:F:178:ASN:ND2	2.46	0.48
1:A:110:LYS:HG3	1:A:111:LYS:HG3	1.96	0.48
1:C:225:ARG:C	1:C:227:LYS:H	2.22	0.48
1:A:236:ILE:HD11	1:A:341:THR:HA	1.94	0.48
1:D:128:VAL:HB	1:D:131:GLN:HG3	1.96	0.48
1:C:149:VAL:HG13	1:C:152:LEU:HB2	1.95	0.48
1:E:90:LYS:C	1:E:92:ASP:H	2.22	0.48
1:D:197:GLN:OE1	1:D:207:ARG:NH1	2.45	0.47
1:A:27:ILE:HG21	1:D:27:ILE:HG21	1.95	0.47
1:F:322:THR:HG22	1:F:327:GLU:HG2	1.96	0.47
1:D:283:ASP:OD2	1:D:286:THR:OG1	2.24	0.47
1:C:251:LEU:HD12	1:C:253:ILE:HG22	1.96	0.47
1:F:227:LYS:O	1:F:227:LYS:HD2	2.15	0.47
1:B:128:VAL:HG12	1:B:131:GLN:HG2	1.96	0.46
1:A:128:VAL:HB	1:A:131:GLN:HG3	1.97	0.46
1:F:173:VAL:HG12	1:F:174:LYS:H	1.80	0.46
1:B:2:SER:HB2	1:F:2:SER:HB2	1.97	0.46
1:A:150:LYS:NZ	1:A:150:LYS:HA	2.31	0.46
1:F:213:ASP:OD2	1:F:226:TYR:OH	2.30	0.46
1:D:174:LYS:O	1:D:175:THR:HG22	2.17	0.45
1:A:110:LYS:HG2	1:A:114:GLU:OE2	2.16	0.45
1:B:182:LYS:HG2	1:B:187:VAL:HG22	1.97	0.45
1:D:182:LYS:HG2	1:D:187:VAL:HG22	1.97	0.45
1:A:5:ASN:HA	1:A:21:GLY:O	2.17	0.45
1:F:226:TYR:C	1:F:227:LYS:HG3	2.43	0.44
1:D:226:TYR:C	1:D:227:LYS:HG3	2.42	0.44
1:C:7:ALA:O	1:C:11:VAL:HG23	2.18	0.44
1:F:139:ARG:HG2	1:F:184:ASP:HA	2.00	0.43
1:C:128:VAL:HB	1:C:131:GLN:HG3	2.00	0.43
1:F:194:TYR:HB2	1:F:323:ILE:HG12	2.00	0.43
1:D:244:SER:O	1:D:288:SER:HA	2.19	0.43
1:E:111:LYS:HG2	1:E:114:GLU:HG3	2.00	0.43
1:B:217:LEU:HB3	1:B:221:GLU:HG3	2.01	0.43
1:E:246:LEU:HD13	1:E:281:ILE:HG13	1.99	0.43
1:A:147:GLY:O	1:A:178:ASN:ND2	2.50	0.43
1:D:139:ARG:HG2	1:D:184:ASP:HA	2.01	0.42
1:B:119:PRO:HG2	1:B:120:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:VAL:O	1:A:334:CYS:HB2	2.20	0.42
1:D:317:LYS:HE2	1:D:332:LEU:HD23	2.01	0.42
1:E:160:GLN:OE1	1:E:160:GLN:N	2.52	0.42
1:F:317:LYS:HE2	1:F:332:LEU:HD23	2.02	0.42
1:B:252:LEU:HA	1:B:255:LEU:HD13	2.02	0.41
1:D:131:GLN:H	1:D:134:LEU:HD23	1.85	0.41
1:A:233:PHE:C	1:A:235:HIS:H	2.28	0.41
1:C:11:VAL:HG12	1:C:12:ASN:H	1.85	0.41
1:E:286:THR:HA	1:F:171:GLU:HG2	2.01	0.41
1:C:2:SER:HB2	1:E:2:SER:HB2	2.02	0.41
1:A:145:THR:HG22	1:A:180:TYR:HE1	1.86	0.41
1:B:251:LEU:HD22	1:B:251:LEU:HA	1.87	0.41
1:D:118:ALA:O	1:D:140:ASN:ND2	2.52	0.41
1:E:197:GLN:OE1	1:E:207:ARG:NH1	2.52	0.41
1:C:111:LYS:HB2	1:C:111:LYS:HE2	1.88	0.40
1:B:160:GLN:N	1:B:160:GLN:OE1	2.54	0.40
1:B:235:HIS:O	1:B:248:GLY:HA3	2.21	0.40
1:D:90:LYS:HD2	1:D:273:ASP:HB2	2.03	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	345/347 (99%)	317 (92%)	23 (7%)	5 (1%)	9 37
1	B	345/347 (99%)	323 (94%)	20 (6%)	2 (1%)	22 57
1	C	345/347 (99%)	322 (93%)	19 (6%)	4 (1%)	11 41
1	D	345/347 (99%)	320 (93%)	21 (6%)	4 (1%)	11 41
1	E	345/347 (99%)	314 (91%)	25 (7%)	6 (2%)	7 33
1	F	345/347 (99%)	328 (95%)	15 (4%)	2 (1%)	22 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2070/2082 (99%)	1924 (93%)	123 (6%)	23 (1%)	12 44

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	ASP
1	A	235	HIS
1	B	269	PHE
1	E	259	PHE
1	C	12	ASN
1	C	37	ASP
1	C	218	ALA
1	F	247	GLY
1	A	20	GLN
1	A	236	ILE
1	B	37	ASP
1	C	247	GLY
1	D	227	LYS
1	D	316	SER
1	D	318	VAL
1	E	316	SER
1	E	261	GLU
1	D	244	SER
1	E	244	SER
1	E	247	GLY
1	A	247	GLY
1	E	28	ILE
1	F	28	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	309/309 (100%)	300 (97%)	9 (3%)	37 70
1	B	309/309 (100%)	301 (97%)	8 (3%)	41 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	309/309 (100%)	299 (97%)	10 (3%)	34 67
1	D	309/309 (100%)	296 (96%)	13 (4%)	25 59
1	E	309/309 (100%)	296 (96%)	13 (4%)	25 59
1	F	309/309 (100%)	302 (98%)	7 (2%)	45 75
All	All	1854/1854 (100%)	1794 (97%)	60 (3%)	34 67

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	148	SER
1	A	150	LYS
1	A	186	VAL
1	A	234	GLU
1	A	251	LEU
1	A	281	ILE
1	A	306	ILE
1	A	314	VAL
1	B	0	HIS
1	B	1	MET
1	B	128	VAL
1	B	143	LEU
1	B	186	VAL
1	B	251	LEU
1	B	292	VAL
1	B	314	VAL
1	C	0	HIS
1	C	1	MET
1	C	20	GLN
1	C	57	GLU
1	C	156	VAL
1	C	176	GLN
1	C	221	GLU
1	C	251	LEU
1	C	261	GLU
1	C	346	LEU
1	D	1	MET
1	D	175	THR
1	D	176	GLN
1	D	189	GLN
1	D	227	LYS

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Mol	Chain	Res	Type
1	D	245	GLN
1	D	253	ILE
1	D	281	ILE
1	D	292	VAL
1	D	306	ILE
1	D	308	LYS
1	D	314	VAL
1	D	317	LYS
1	E	1	MET
1	E	148	SER
1	E	176	GLN
1	E	183	VAL
1	E	189	GLN
1	E	192	GLU
1	E	196	THR
1	E	252	LEU
1	E	253	ILE
1	E	261	GLU
1	E	281	ILE
1	E	286	THR
1	E	315	VAL
1	F	65	LYS
1	F	173	VAL
1	F	189	GLN
1	F	192	GLU
1	F	234	GLU
1	F	253	ILE
1	F	281	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	B	164	ASN
1	C	15	HIS
1	C	30	ASN
1	C	164	ASN
1	C	176	GLN
1	C	278	ASN
1	D	176	GLN
1	E	15	HIS
1	E	176	GLN

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Mol	Chain	Res	Type
1	E	188	GLN
1	F	30	ASN
1	F	176	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 oligosaccharides 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	347/347 (100%)	-2.07	0	100	100	46, 69, 99, 133	0
1	B	347/347 (100%)	-2.08	0	100	100	45, 69, 101, 150	0
1	C	347/347 (100%)	-2.08	0	100	100	41, 70, 102, 136	0
1	D	347/347 (100%)	-2.07	0	100	100	47, 74, 119, 152	0
1	E	347/347 (100%)	-2.04	0	100	100	39, 73, 126, 164	0
1	F	347/347 (100%)	-2.06	0	100	100	44, 74, 115, 151	0
All	All	2082/2082 (100%)	-2.07	0	100	100	39, 72, 113, 164	0

There are no RSRZ outliers to report.

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 monosaccharides 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.