



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2021 – 11:38 AM EST

PDB ID : 6WUU
Title : Crystal structure of the SARS CoV-2 Papain-like protease in complex with peptide inhibitor VIR250
Authors : Lv, Z.; Olsen, S.K.
Deposited on : 2020-05-05
Resolution : 2.79 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

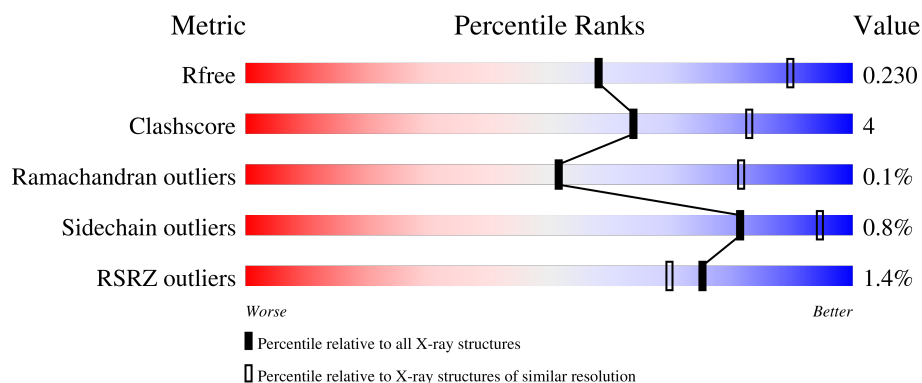
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 $\leq 5\%$. 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	326	<div> <div>2%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	B	326	<div> <div>%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	C	326	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	D	326	<div> <div>%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
2	G	5	<div> <div>60%</div> <div>20%</div> <div>20%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	5	
2	I	5	
2	J	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GVE	G	5	-	X	-	-
2	GVE	H	5	-	X	-	-
2	GVE	I	5	-	X	-	-
2	GVE	J	5	-	X	-	-
4	MG	C	502	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10292 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 Non-structural protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2527	1608	419	480	20			
1	B	321	Total	C	N	O	S	0	0	0
			2554	1625	424	485	20			
1	C	317	Total	C	N	O	S	0	0	0
			2516	1603	415	479	19			
1	D	318	Total	C	N	O	S	0	0	0
			2525	1608	416	482	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P0DTD1
A	317	LEU	-	expression tag	UNP P0DTD1
A	318	GLU	-	expression tag	UNP P0DTD1
A	319	HIS	-	expression tag	UNP P0DTD1
A	320	HIS	-	expression tag	UNP P0DTD1
A	321	HIS	-	expression tag	UNP P0DTD1
A	322	HIS	-	expression tag	UNP P0DTD1
A	323	HIS	-	expression tag	UNP P0DTD1
A	324	HIS	-	expression tag	UNP P0DTD1
B	-1	MET	-	initiating methionine	UNP P0DTD1
B	317	LEU	-	expression tag	UNP P0DTD1
B	318	GLU	-	expression tag	UNP P0DTD1
B	319	HIS	-	expression tag	UNP P0DTD1
B	320	HIS	-	expression tag	UNP P0DTD1
B	321	HIS	-	expression tag	UNP P0DTD1
B	322	HIS	-	expression tag	UNP P0DTD1
B	323	HIS	-	expression tag	UNP P0DTD1
B	324	HIS	-	expression tag	UNP P0DTD1
C	-1	MET	-	initiating methionine	UNP P0DTD1
C	317	LEU	-	expression tag	UNP P0DTD1
C	318	GLU	-	expression tag	UNP P0DTD1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	319	HIS	-	expression tag	UNP P0DTD1
C	320	HIS	-	expression tag	UNP P0DTD1
C	321	HIS	-	expression tag	UNP P0DTD1
C	322	HIS	-	expression tag	UNP P0DTD1
C	323	HIS	-	expression tag	UNP P0DTD1
C	324	HIS	-	expression tag	UNP P0DTD1
D	-1	MET	-	initiating methionine	UNP P0DTD1
D	317	LEU	-	expression tag	UNP P0DTD1
D	318	GLU	-	expression tag	UNP P0DTD1
D	319	HIS	-	expression tag	UNP P0DTD1
D	320	HIS	-	expression tag	UNP P0DTD1
D	321	HIS	-	expression tag	UNP P0DTD1
D	322	HIS	-	expression tag	UNP P0DTD1
D	323	HIS	-	expression tag	UNP P0DTD1
D	324	HIS	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called VIR250.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	5	Total	C	N	O	S	0	0	0
			36	23	6	6	1			
2	H	5	Total	C	N	O	S	0	0	0
			36	23	6	6	1			
2	I	5	Total	C	N	O	S	0	0	0
			36	23	6	6	1			
2	J	5	Total	C	N	O	S	0	0	0
			36	23	6	6	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	D	2	Total 2	Mg 2	0	0
4	C	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

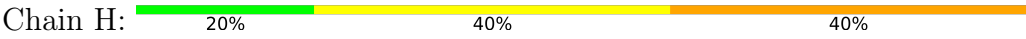
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	B	9	Total 9	O 9	0	0
5	C	1	Total 1	O 1	0	0
5	D	5	Total 5	O 5	0	0



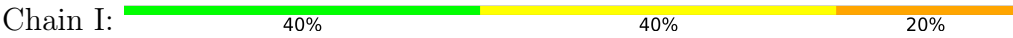
● Molecule 2: VIR250



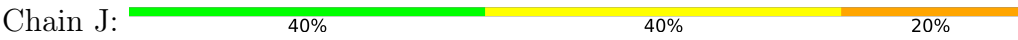
● Molecule 2: VIR250



● Molecule 2: VIR250



● Molecule 2: VIR250



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.42Å 189.69Å 63.12Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	94.85 – 2.79 94.85 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (94.85-2.79) 91.7 (94.85-2.79)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.195 , 0.230 0.195 , 0.230	Depositor DCC
R_{free} test set	1993 reflections (5.95%)	wwPDB-VP
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10292	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UB4, ZN, ACE, DPP, MG, GVE

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	0/2587	0.48	0/3509
1	B	0.28	0/2615	0.48	0/3547
1	C	0.28	0/2576	0.46	0/3496
1	D	0.28	0/2585	0.46	0/3508
2	G	2.28	0/3	0.39	0/2
2	H	2.37	0/3	0.59	0/2
2	I	2.14	0/3	0.43	0/2
2	J	2.51	0/3	0.34	0/2
All	All	0.29	0/10375	0.47	0/14068

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 [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	2527	0	2475	24	0
1	B	2554	0	2499	24	1
1	C	2516	0	2464	18	1
1	D	2525	0	2470	22	0
2	G	36	0	20	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	36	0	19	4	0
2	I	36	0	20	3	0
2	J	36	0	20	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	3	0	0	0	0
5	B	9	0	0	0	0
5	C	1	0	0	0	0
5	D	5	0	0	0	0
All	All	10292	0	9987	85	1

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 4.

All (85) 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:C:111:CYS:H	2:I:5:GVE:HB1	1.35	0.92
1:D:111:CYS:H	2:J:5:GVE:HB1	1.51	0.76
1:D:101:LEU:HD23	1:D:140:ARG:HH12	1.52	0.73
1:C:101:LEU:HD23	1:C:140:ARG:HH12	1.56	0.71
1:A:111:CYS:H	2:G:5:GVE:HB1	1.55	0.71
1:D:267:ASN:OD1	1:D:270:CYS:N	2.19	0.69
1:A:166:ARG:NH2	1:C:167:GLU:OE1	2.25	0.68
1:B:218:LYS:N	1:B:218:LYS:HD2	2.11	0.64
1:D:101:LEU:HA	1:D:140:ARG:HH12	1.63	0.63
1:A:254:LYS:HD2	1:B:266:GLY:HA2	1.79	0.63
1:B:33:PRO:HB2	1:B:58:LEU:HD13	1.82	0.61
1:A:33:PRO:HB2	1:A:58:LEU:HD13	1.82	0.61
1:D:189:CYS:HB3	1:D:192:CYS:HB2	1.82	0.61
1:D:312:THR:OG1	1:D:314:ILE:HG12	2.01	0.60
1:B:61:ASP:OD2	1:B:63:THR:OG1	2.16	0.60
1:B:188:VAL:HG22	1:B:194:GLN:HG3	1.82	0.59
1:D:101:LEU:HA	1:D:140:ARG:NH1	2.19	0.56
1:B:33:PRO:HG2	1:B:58:LEU:HD22	1.87	0.56
1:A:60:ASN:OD1	1:A:61:ASP:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:CYS:HB3	1:C:291:THR:HB	1.89	0.55
1:C:106:TRP:CD1	1:C:106:TRP:N	2.67	0.55
1:D:208:MET:HE2	2:H:1:ACE:H3	1.88	0.55
1:C:106:TRP:H	1:C:106:TRP:HD1	1.53	0.54
1:D:138:ARG:HD3	1:D:143:GLU:OE1	2.07	0.54
1:B:280:GLU:OE2	1:B:283:TYR:OH	2.21	0.53
1:A:310:TYR:HE1	1:B:289:LEU:HB3	1.74	0.53
1:B:189:CYS:HB3	1:B:192:CYS:HB2	1.91	0.53
1:D:317:LEU:HD12	1:D:317:LEU:H	1.74	0.53
1:D:101:LEU:HD23	1:D:140:ARG:NH1	2.24	0.52
1:A:157:LYS:NZ	1:A:162:LEU:O	2.43	0.51
1:B:214:GLU:CD	1:B:218:LYS:HZ1	2.14	0.51
1:D:234:LEU:HD21	1:D:237:GLN:HB2	1.93	0.50
1:B:317:LEU:HD12	1:B:317:LEU:O	2.12	0.49
1:C:264:TYR:CZ	1:C:271:GLY:HA3	2.48	0.48
1:C:314:ILE:HG22	1:C:316:PRO:HD3	1.95	0.48
1:B:283:TYR:HD2	1:B:290:LEU:HD11	1.77	0.48
1:A:315:LYS:HG2	1:A:316:PRO:HD2	1.95	0.47
1:C:111:CYS:N	2:I:5:GVE:HB1	2.11	0.47
1:B:183:ARG:HD3	1:B:185:LEU:HD21	1.95	0.47
1:C:8:PHE:HE1	1:C:18:THR:HG1	1.63	0.47
1:A:152:LEU:HD13	1:A:159:VAL:HG22	1.97	0.47
1:B:120:LEU:O	1:B:136:TYR:OH	2.32	0.47
1:A:11:VAL:HG13	1:A:64:LEU:HD22	1.97	0.47
1:D:226:CYS:SG	1:D:227:GLY:N	2.88	0.46
1:C:189:CYS:HB3	1:C:192:CYS:HB2	1.97	0.46
1:A:33:PRO:HG2	1:A:58:LEU:HD22	1.98	0.46
1:B:272:HIS:ND1	2:H:5:GVE:HG2	2.31	0.46
1:D:11:VAL:HG13	1:D:64:LEU:HD22	1.98	0.46
1:C:62:ASP:OD1	1:C:65:ARG:NH1	2.48	0.46
1:A:222:ILE:HA	1:A:222:ILE:HD13	1.90	0.45
1:A:157:LYS:HE3	1:A:157:LYS:HB3	1.81	0.45
1:A:166:ARG:HA	1:A:243:MET:HE1	1.99	0.45
1:B:208:MET:HE2	2:J:1:ACE:H3	1.99	0.45
1:D:283:TYR:CE2	1:D:292:LYS:HG2	2.52	0.45
1:D:152:LEU:HD13	1:D:159:VAL:HG22	1.98	0.44
1:A:119:THR:HG21	1:A:304:PHE:CZ	2.53	0.44
1:A:264:TYR:CZ	1:A:271:GLY:HA3	2.53	0.44
1:D:213:TYR:HB2	1:D:305:TYR:CE2	2.53	0.44
1:B:12:ASP:OD2	1:B:12:ASP:N	2.52	0.43
1:C:165:VAL:O	1:C:169:MET:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:TYR:CE2	1:D:300:ILE:HD11	2.53	0.43
1:A:221:GLN:HB3	1:A:229:GLN:HE21	1.84	0.43
1:B:162:LEU:HB3	2:H:3:DPP:C	2.49	0.43
1:A:234:LEU:HD21	1:A:237:GLN:HB2	2.01	0.43
1:A:12:ASP:OD2	1:A:12:ASP:N	2.52	0.43
1:B:128:ASN:HB2	1:B:129:PRO:HD3	2.01	0.42
1:B:264:TYR:CZ	1:B:271:GLY:HA3	2.54	0.42
1:C:192:CYS:SG	1:C:226:CYS:HB3	2.58	0.42
1:B:147:PHE:CE2	1:B:151:ILE:HD11	2.54	0.42
1:A:164:ASP:HB3	1:A:167:GLU:HB3	2.00	0.42
1:B:61:ASP:OD2	1:B:63:THR:N	2.46	0.42
1:C:106:TRP:CD1	1:C:287:GLY:HA3	2.55	0.42
1:A:315:LYS:CG	1:A:316:PRO:HD2	2.49	0.42
1:B:164:ASP:OD1	2:H:2:UB4:N	2.52	0.41
1:A:165:VAL:O	1:A:169:MET:HG2	2.20	0.41
1:D:283:TYR:HD2	1:D:290:LEU:HD11	1.85	0.41
1:A:189:CYS:HB3	1:A:192:CYS:HB2	2.03	0.41
1:D:157:LYS:NZ	1:D:163:GLY:HA2	2.36	0.41
1:D:33:PRO:HA	1:D:42:THR:OG1	2.21	0.41
1:C:170:SER:O	1:C:174:GLN:HG2	2.21	0.41
1:A:22:ASP:OD2	1:A:24:SER:OG	2.39	0.41
1:D:264:TYR:CZ	1:D:271:GLY:HA3	2.57	0.40
1:B:13:ASN:HB2	1:B:56:TYR:OH	2.21	0.40
1:C:28:GLY:HA2	1:C:32:GLY:O	2.21	0.40
1:C:162:LEU:HB3	2:I:3:DPP:C	2.51	0.40

All (1) 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:B:3:ARG:NH1	1:C:1:GLU:OE2[2_744]	2.00	0.20

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	316/326 (97%)	302 (96%)	13 (4%)	1 (0%)	41	72
1	B	319/326 (98%)	305 (96%)	14 (4%)	0	100	100
1	C	315/326 (97%)	300 (95%)	15 (5%)	0	100	100
1	D	316/326 (97%)	300 (95%)	16 (5%)	0	100	100
2	G	1/5 (20%)	1 (100%)	0	0	100	100
2	H	1/5 (20%)	1 (100%)	0	0	100	100
2	I	1/5 (20%)	1 (100%)	0	0	100	100
2	J	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1270/1324 (96%)	1211 (95%)	58 (5%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	LYS

5.3.2 Protein sidechains ⓘ

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	278/286 (97%)	277 (100%)	1 (0%)	91	97
1	B	281/286 (98%)	277 (99%)	4 (1%)	67	90
1	C	277/286 (97%)	276 (100%)	1 (0%)	91	97
1	D	278/286 (97%)	275 (99%)	3 (1%)	73	92
All	All	1114/1144 (97%)	1105 (99%)	9 (1%)	81	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	0	ARG
1	B	106	TRP
1	B	315	LYS
1	B	319	HIS
1	C	106	TRP
1	D	315	LYS
1	D	317	LEU
1	D	318	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DPP	J	3	2	3,5,6	0.75	0	1,5,7	0.30	0
2	DPP	H	3	2	3,5,6	0.79	0	1,5,7	0.20	0
2	DPP	I	3	2	3,5,6	0.70	0	1,5,7	0.19	0
2	GVE	H	5	1,2	7,7,7	1.12	0	7,7,7	3.45	4 (57%)
2	GVE	J	5	1,2	7,7,7	1.25	0	7,7,7	3.43	4 (57%)
2	UB4	G	2	2	13,16,17	1.55	1 (7%)	9,21,23	2.20	3 (33%)
2	UB4	H	2	2	13,16,17	1.58	1 (7%)	9,21,23	1.98	3 (33%)
2	UB4	I	2	2	13,16,17	1.65	1 (7%)	9,21,23	2.19	3 (33%)
2	UB4	J	2	2	13,16,17	1.54	1 (7%)	9,21,23	2.21	3 (33%)
2	DPP	G	3	2	3,5,6	0.83	0	1,5,7	0.29	0
2	GVE	G	5	1,2	7,7,7	1.33	1 (14%)	7,7,7	3.43	4 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GVE	I	5	1,2	7,7,7	1.34	1 (14%)	7,7,7	3.44	3 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DPP	J	3	2	-	1/2/4/6	-
2	DPP	H	3	2	-	1/2/4/6	-
2	DPP	I	3	2	-	1/2/4/6	-
2	GVE	H	5	1,2	-	5/6/6/6	-
2	GVE	J	5	1,2	-	5/6/6/6	-
2	UB4	G	2	2	-	1/5/7/9	0/2/2/2
2	UB4	H	2	2	-	2/5/7/9	0/2/2/2
2	UB4	I	2	2	-	2/5/7/9	0/2/2/2
2	UB4	J	2	2	-	1/5/7/9	0/2/2/2
2	DPP	G	3	2	-	1/2/4/6	-
2	GVE	G	5	1,2	-	5/6/6/6	-
2	GVE	I	5	1,2	-	5/6/6/6	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	UB4	CG-CD	4.81	1.52	1.49
2	H	2	UB4	CG-CD	4.52	1.52	1.49
2	G	2	UB4	CG-CD	4.40	1.52	1.49
2	J	2	UB4	CG-CD	4.32	1.52	1.49
2	I	5	GVE	OE1-CH3	-2.24	1.40	1.45
2	G	5	GVE	OE1-CH3	-2.07	1.40	1.45

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	5	GVE	CA-CB-CG	7.06	133.78	112.84
2	H	5	GVE	CA-CB-CG	6.95	133.47	112.84
2	J	5	GVE	CA-CB-CG	6.75	132.88	112.84
2	G	5	GVE	CA-CB-CG	6.66	132.60	112.84
2	J	2	UB4	CZ1-CZ2-SE1	-4.60	105.75	111.85
2	I	2	UB4	CZ1-CZ2-SE1	-4.55	105.82	111.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	UB4	CZ1-CZ2-SE1	-4.48	105.91	111.85
2	G	5	GVE	CB-CG-CD	4.03	128.27	113.62
2	G	5	GVE	OE1-CD-OE2	-3.93	110.83	123.14
2	J	5	GVE	CB-CG-CD	3.91	127.83	113.62
2	H	5	GVE	OE1-CD-OE2	-3.89	110.96	123.14
2	H	2	UB4	CZ1-CZ2-SE1	-3.87	106.72	111.85
2	J	5	GVE	OE1-CD-OE2	-3.86	111.04	123.14
2	J	2	UB4	CZ2-CZ1-NE1	3.84	116.98	108.04
2	G	2	UB4	CZ2-CZ1-NE1	3.84	116.97	108.04
2	I	5	GVE	CB-CG-CD	3.76	127.29	113.62
2	I	5	GVE	OE1-CD-OE2	-3.73	111.46	123.14
2	I	2	UB4	CZ2-CZ1-NE1	3.72	116.69	108.04
2	H	5	GVE	CB-CG-CD	3.45	126.17	113.62
2	H	2	UB4	CZ2-CZ1-NE1	3.40	115.95	108.04
2	H	5	GVE	OE1-CD-CG	2.78	123.21	112.23
2	I	2	UB4	CT1-CZ1-NE1	-2.67	123.05	130.78
2	G	2	UB4	CT1-CZ1-NE1	-2.61	123.20	130.78
2	J	2	UB4	CT1-CZ1-NE1	-2.58	123.31	130.78
2	H	2	UB4	CT1-CZ1-NE1	-2.53	123.43	130.78
2	J	5	GVE	OE1-CD-CG	2.41	121.75	112.23
2	G	5	GVE	OE1-CD-CG	2.18	120.84	112.23

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	3	DPP	N-CA-CB-NG
2	H	3	DPP	N-CA-CB-NG
2	I	3	DPP	N-CA-CB-NG
2	H	5	GVE	CA-CB-CG-CD
2	J	5	GVE	CA-CB-CG-CD
2	G	2	UB4	C-CA-CB-CG
2	H	2	UB4	C-CA-CB-CG
2	I	2	UB4	C-CA-CB-CG
2	J	2	UB4	C-CA-CB-CG
2	G	3	DPP	N-CA-CB-NG
2	G	5	GVE	CA-CB-CG-CD
2	I	5	GVE	CA-CB-CG-CD
2	H	5	GVE	CG-CD-OE1-CH3
2	J	5	GVE	CG-CD-OE1-CH3
2	G	5	GVE	CG-CD-OE1-CH3
2	J	5	GVE	OE2-CD-OE1-CH3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	5	GVE	OE2-CD-OE1-CH3
2	H	5	GVE	OE2-CD-OE1-CH3
2	I	5	GVE	CG-CD-OE1-CH3
2	I	5	GVE	OE1-CD-CG-CB
2	J	5	GVE	OE1-CD-CG-CB
2	G	5	GVE	OE1-CD-CG-CB
2	H	5	GVE	OE1-CD-CG-CB
2	I	5	GVE	OE2-CD-OE1-CH3
2	H	5	GVE	N-CA-CB-CG
2	J	5	GVE	N-CA-CB-CG
2	I	5	GVE	N-CA-CB-CG
2	G	5	GVE	N-CA-CB-CG
2	H	2	UB4	N-CA-CB-CG
2	I	2	UB4	N-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	3	DPP	1	0
2	I	3	DPP	1	0
2	H	5	GVE	1	0
2	J	5	GVE	1	0
2	H	2	UB4	1	0
2	G	5	GVE	1	0
2	I	5	GVE	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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, 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	318/326 (97%)	0.17	6 (1%) 66 59	47, 77, 117, 147	0
1	B	321/326 (98%)	0.10	3 (0%) 84 80	51, 72, 115, 136	0
1	C	317/326 (97%)	0.18	5 (1%) 72 66	53, 77, 122, 148	0
1	D	318/326 (97%)	0.19	4 (1%) 77 72	51, 76, 125, 164	0
2	G	1/5 (20%)	-0.86	0 100 100	62, 62, 62, 62	0
2	H	1/5 (20%)	-0.25	0 100 100	72, 72, 72, 72	0
2	I	1/5 (20%)	0.07	0 100 100	64, 64, 64, 64	0
2	J	1/5 (20%)	0.08	0 100 100	52, 52, 52, 52	0
All	All	1278/1324 (96%)	0.16	18 (1%) 75 70	47, 76, 119, 164	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	MET	6.1
1	D	137	TYR	3.9
1	D	106	TRP	3.6
1	C	296	TYR	3.4
1	A	191	THR	3.2
1	A	106	TRP	3.1
1	B	-1	MET	2.6
1	C	137	TYR	2.5
1	A	1	GLU	2.5
1	B	268	TYR	2.4
1	A	0	ARG	2.4
1	C	297	LYS	2.3
1	B	43	LYS	2.3
1	D	268	TYR	2.2
1	C	1	GLU	2.1
1	C	3	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	185	LEU	2.0
1	A	268	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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	UB4	H	2	15/16	0.85	0.32	76,88,98,99	0
2	DPP	H	3	6/7	0.87	0.15	69,72,79,85	0
2	UB4	I	2	15/16	0.88	0.20	70,77,91,95	0
2	DPP	I	3	6/7	0.91	0.16	59,80,84,85	0
2	UB4	G	2	15/16	0.91	0.22	70,79,88,91	0
2	GVE	J	5	8/8	0.93	0.19	54,77,85,87	0
2	GVE	H	5	8/8	0.94	0.22	56,73,92,97	0
2	UB4	J	2	15/16	0.94	0.18	61,79,93,96	0
2	GVE	I	5	8/8	0.94	0.23	65,79,93,97	0
2	GVE	G	5	8/8	0.95	0.14	71,85,89,89	0
2	DPP	G	3	6/7	0.95	0.16	71,77,81,87	0
2	DPP	J	3	6/7	0.97	0.14	64,67,70,70	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95th 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
3	ZN	D	501	1/1	0.44	0.15	207,207,207,207	0
4	MG	C	502	1/1	0.79	0.69	120,120,120,120	0
4	MG	D	502	1/1	0.91	0.12	52,52,52,52	0
4	MG	D	503	1/1	0.91	0.60	108,108,108,108	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	B	502	1/1	0.94	0.22	60,60,60,60	0
3	ZN	C	501	1/1	0.95	0.14	119,119,119,119	0
3	ZN	B	501	1/1	0.96	0.11	106,106,106,106	0
3	ZN	A	501	1/1	0.98	0.12	108,108,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.