



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 11:18 AM JST

PDB ID : 7F2E
Title : SARS-CoV-2 nucleocapsid protein C-terminal domain (dodecamer)
Authors : Liu, C.; Jiang, H.
Deposited on : 2021-06-10
Resolution : 3.10 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

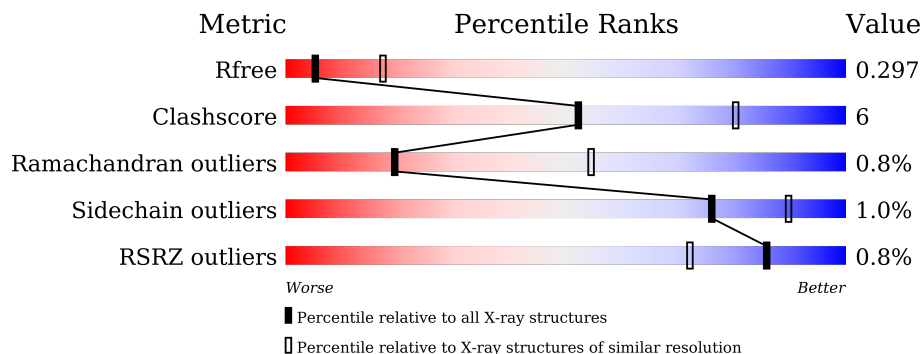
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	108	 90% 8% .
1	B	108	 86% 11% ..
1	C	108	 92% 7% .
1	D	108	 81% 18% .
1	E	108	 76% 12% . 11%
1	F	108	 79% 10% . 10%

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Mol	Chain	Length	Quality of chain
1	G	108	 84% 15%
1	H	108	 79% 19%
1	I	108	 83% 16%
1	J	108	 86% 12%
1	K	108	 73% 15% 11%
1	L	108	 76% 9% 15%

2 Entry composition

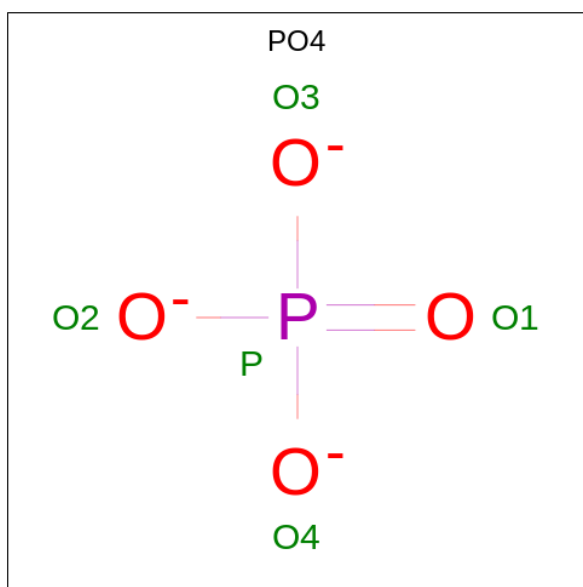
There are 3 unique types of molecules in this entry. The entry contains 8752 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	106	Total 789	C 504	N 143	O 140	S 2	0	0	0
1	A	106	Total 776	C 491	N 141	O 142	S 2	0	0	0
1	C	107	Total 799	C 508	N 143	O 146	S 2	0	0	0
1	D	107	Total 784	C 497	N 141	O 144	S 2	0	0	0
1	E	96	Total 608	C 384	N 109	O 113	S 2	0	0	0
1	F	97	Total 616	C 384	N 116	O 115	S 1	0	0	0
1	G	107	Total 824	C 520	N 148	O 154	S 2	0	0	0
1	H	106	Total 768	C 490	N 137	O 139	S 2	0	0	0
1	I	107	Total 808	C 515	N 148	O 143	S 2	0	0	0
1	J	106	Total 764	C 484	N 138	O 140	S 2	0	0	0
1	K	96	Total 602	C 378	N 113	O 109	S 2	0	0	0
1	L	92	Total 592	C 368	N 110	O 112	S 2	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		

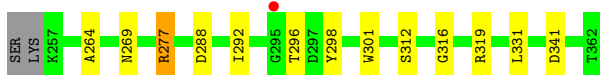
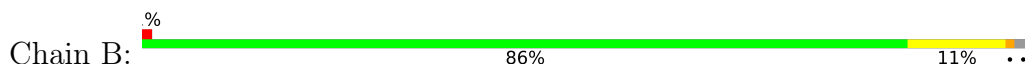
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		
3	G	1	Total	O	0	0
			1	1		

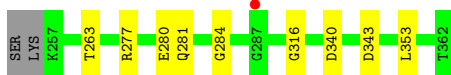
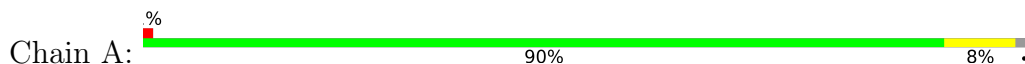
3 Residue-property plots [i](#)

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.

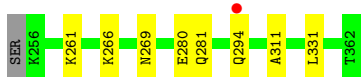
- Molecule 1: Nucleoprotein



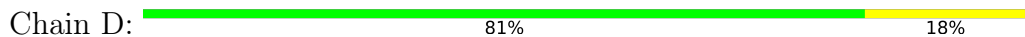
- Molecule 1: Nucleoprotein



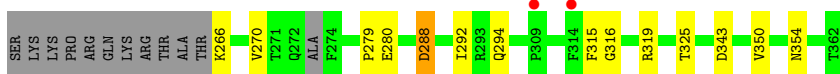
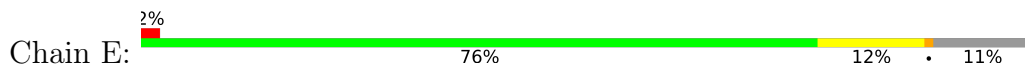
- Molecule 1: Nucleoprotein




- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein




- Molecule 1: Nucleoprotein

Chain F:  79% 10% 10%




• Molecule 1: Nucleoprotein

Chain G:  84% 15%




• Molecule 1: Nucleoprotein

Chain H:  79% 19%




• Molecule 1: Nucleoprotein

Chain I:  83% 16%



• Molecule 1: Nucleoprotein

Chain J:  86% 12%




• Molecule 1: Nucleoprotein

Chain K:  73% 15% 11% 2%



• Molecule 1: Nucleoprotein

Chain L:  76% 9% 15% 2%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	102.54Å 102.54Å 389.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.84 – 3.10 38.58 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.84-3.10) 95.9 (38.58-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.14_3247	Depositor
R, R_{free}	0.268 , 0.297 0.268 , 0.297	Depositor DCC
R_{free} test set	1376 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtrriage
Anisotropy	0.208	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.470 for -h-k,k,-l	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8752	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.97% 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: PO4

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	0.24	0/795	0.40	0/1079
1	B	0.25	0/809	0.41	0/1099
1	C	0.25	0/818	0.40	0/1107
1	D	0.25	0/804	0.40	0/1094
1	E	0.24	0/621	0.41	0/850
1	F	0.24	0/625	0.41	0/851
1	G	0.24	0/845	0.40	0/1146
1	H	0.24	0/788	0.41	0/1075
1	I	0.24	0/828	0.39	0/1121
1	J	0.24	0/785	0.40	0/1070
1	K	0.24	0/613	0.42	0/834
1	L	0.24	0/602	0.41	0/819
All	All	0.24	0/8933	0.41	0/12145

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	776	0	676	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	789	0	717	11	0
1	C	799	0	718	6	0
1	D	784	0	688	13	0
1	E	608	0	426	10	0
1	F	616	0	446	8	0
1	G	824	0	769	13	0
1	H	768	0	672	14	0
1	I	808	0	752	12	0
1	J	764	0	648	12	0
1	K	602	0	414	10	0
1	L	592	0	418	8	0
2	G	10	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
3	B	1	0	0	0	0
3	G	1	0	0	0	0
All	All	8752	0	7344	89	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 (89) 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:K:350:VAL:O	1:K:354:ASN:ND2	2.25	0.70
1:I:256:LYS:HD3	1:I:257:LYS:H	1.59	0.68
1:F:298:TYR:HB3	1:F:301:TRP:HB2	1.76	0.67
1:E:316:GLY:O	1:F:277:ARG:NH2	2.29	0.65
1:E:350:VAL:O	1:E:354:ASN:ND2	2.25	0.65
1:F:280:GLU:HB2	1:F:283:GLN:HG3	1.78	0.64
1:K:280:GLU:O	1:L:319:ARG:NH1	2.31	0.64
1:C:266:LYS:HG3	1:C:294:GLN:HA	1.82	0.62
1:C:281:GLN:HA	1:D:319:ARG:HD2	1.83	0.60
1:B:331:LEU:HD13	1:A:353:LEU:HD13	1.83	0.60
1:G:280:GLU:O	1:H:319:ARG:NH1	2.37	0.58
1:L:280:GLU:HB2	1:L:283:GLN:HG3	1.86	0.57
1:H:269:ASN:HB2	1:H:292:ILE:O	2.04	0.57
1:I:331:LEU:HD13	1:J:353:LEU:HD13	1.85	0.56
1:C:331:LEU:HD13	1:D:353:LEU:HD13	1.87	0.56
1:G:331:LEU:HD13	1:H:353:LEU:HD13	1.86	0.56
1:C:261:LYS:NZ	1:D:308:ALA:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:GLU:O	1:F:319:ARG:NH1	2.41	0.54
1:D:362:THR:OG1	1:G:289:GLN:NE2	2.41	0.54
1:I:269:ASN:HB2	1:I:292:ILE:O	2.07	0.54
1:H:287:GLY:HA2	1:H:291:LEU:HD23	1.89	0.54
1:J:287:GLY:H	1:J:356:HIS:HB3	1.71	0.54
1:B:319:ARG:HD2	1:A:281:GLN:HA	1.90	0.53
1:K:275:GLY:O	1:K:277:ARG:NH2	2.35	0.53
1:K:266:LYS:N	1:K:294:GLN:O	2.42	0.53
1:H:265:THR:N	1:H:268:TYR:O	2.38	0.53
1:G:281:GLN:HA	1:H:319:ARG:HD2	1.91	0.52
1:E:266:LYS:N	1:E:294:GLN:O	2.42	0.52
1:I:298:TYR:HB3	1:I:301:TRP:HB2	1.93	0.51
1:I:316:GLY:O	1:J:277:ARG:NH1	2.43	0.50
1:I:280:GLU:O	1:J:319:ARG:NH1	2.45	0.50
1:I:281:GLN:HA	1:J:319:ARG:HD2	1.94	0.49
1:A:340:ASP:HB3	1:A:343:ASP:HB2	1.94	0.49
1:G:316:GLY:O	1:H:277:ARG:NH1	2.40	0.49
1:K:309:PRO:HA	1:L:260:GLN:O	2.12	0.49
1:D:269:ASN:HB2	1:D:292:ILE:O	2.13	0.49
1:D:288:ASP:OD1	1:D:289:GLN:N	2.45	0.49
1:B:269:ASN:HB2	1:B:292:ILE:O	2.13	0.49
1:B:316:GLY:O	1:A:277:ARG:NH2	2.46	0.48
1:C:280:GLU:O	1:D:319:ARG:NH1	2.47	0.48
1:A:277:ARG:HH21	1:A:284:GLY:HA3	1.79	0.48
1:K:288:ASP:O	1:K:292:ILE:HG13	2.12	0.48
1:I:319:ARG:NH1	1:J:280:GLU:O	2.47	0.47
1:J:319:ARG:HB2	1:J:334:THR:HG22	1.96	0.47
1:K:283:GLN:O	1:L:319:ARG:NH1	2.46	0.47
1:D:289:GLN:HG3	1:G:289:GLN:HG3	1.95	0.47
1:B:341:ASP:OD1	1:B:341:ASP:N	2.48	0.46
1:I:313:ALA:O	1:I:317:MET:HG2	2.16	0.46
1:D:270:VAL:HG13	1:D:274:PHE:HD2	1.81	0.46
1:L:262:ARG:HB2	1:L:274:PHE:CE1	2.51	0.46
1:G:313:ALA:O	1:G:317:MET:HG2	2.17	0.45
1:B:298:TYR:HB3	1:B:301:TRP:HB2	1.99	0.45
1:G:277:ARG:NH1	1:H:316:GLY:O	2.35	0.45
1:E:279:PRO:HB2	1:L:280:GLU:HG2	1.98	0.44
1:B:288:ASP:O	1:B:292:ILE:HG13	2.18	0.44
1:F:258:PRO:O	1:F:262:ARG:HG3	2.17	0.44
1:B:264:ALA:O	1:B:296:THR:N	2.42	0.43
1:E:319:ARG:NH1	1:F:280:GLU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:SER:HB3	1:A:263:THR:HA	2.01	0.43
1:C:269:ASN:OD1	1:C:269:ASN:N	2.52	0.43
1:H:306:GLN:OE1	1:H:349:GLN:NE2	2.49	0.43
1:H:340:ASP:HB3	1:H:343:ASP:HB2	2.00	0.43
1:D:298:TYR:HB3	1:D:301:TRP:HB2	2.00	0.42
1:B:319:ARG:NH1	1:A:280:GLU:O	2.52	0.42
1:E:315:PHE:HB3	1:F:286:PHE:CD1	2.55	0.42
1:H:264:ALA:O	1:H:296:THR:N	2.36	0.42
1:D:314:PHE:O	1:D:318:SER:OG	2.28	0.42
1:E:270:VAL:HB	1:E:292:ILE:HG23	2.01	0.42
1:I:319:ARG:NH1	1:J:283:GLN:O	2.51	0.42
1:B:277:ARG:HH12	1:A:316:GLY:HA2	1.85	0.42
1:E:319:ARG:HD2	1:F:281:GLN:HA	2.02	0.42
1:G:357:ILE:HD13	1:H:321:GLY:HA2	2.02	0.42
1:G:270:VAL:HG13	1:G:274:PHE:HD2	1.85	0.41
1:K:319:ARG:NH1	1:L:280:GLU:O	2.54	0.41
1:D:264:ALA:O	1:D:296:THR:N	2.39	0.41
1:D:341:ASP:HA	1:D:346:PHE:CG	2.56	0.41
1:E:288:ASP:O	1:E:292:ILE:HG13	2.20	0.41
1:I:357:ILE:HD13	1:J:321:GLY:HA2	2.03	0.41
1:G:330:TRP:CZ3	1:H:338:LYS:HB2	2.56	0.41
1:G:308:ALA:HA	1:G:309:PRO:HD3	1.94	0.40
1:J:321:GLY:O	1:J:332:THR:N	2.51	0.40
1:I:352:LEU:O	1:I:356:HIS:HD2	2.04	0.40
1:J:313:ALA:O	1:J:317:MET:HG2	2.20	0.40
1:K:287:GLY:N	1:K:356:HIS:HB3	2.36	0.40
1:L:258:PRO:O	1:L:262:ARG:HG3	2.21	0.40
1:G:256:LYS:HE2	1:G:257:LYS:HG2	2.03	0.40
1:J:352:LEU:O	1:J:356:HIS:HD2	2.04	0.40
1:K:270:VAL:HB	1:K:292:ILE:HG23	2.02	0.40
1:H:313:ALA:O	1:H:317:MET:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	104/108 (96%)	97 (93%)	7 (7%)	0	100	100
1	B	104/108 (96%)	103 (99%)	1 (1%)	0	100	100
1	C	105/108 (97%)	100 (95%)	4 (4%)	1 (1%)	15	49
1	D	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	E	92/108 (85%)	84 (91%)	6 (6%)	2 (2%)	6	29
1	F	89/108 (82%)	77 (86%)	9 (10%)	3 (3%)	3	21
1	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	H	104/108 (96%)	97 (93%)	7 (7%)	0	100	100
1	I	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
1	J	104/108 (96%)	100 (96%)	4 (4%)	0	100	100
1	K	92/108 (85%)	84 (91%)	7 (8%)	1 (1%)	14	46
1	L	86/108 (80%)	80 (93%)	3 (4%)	3 (4%)	3	20
All	All	1195/1296 (92%)	1120 (94%)	65 (5%)	10 (1%)	19	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	343	ASP
1	L	301	TRP
1	C	311	ALA
1	F	325	THR
1	F	340	ASP
1	L	302	PRO
1	K	325	THR
1	L	325	THR
1	E	325	THR
1	F	258	PRO

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	65/90 (72%)	65 (100%)	0	100	100
1	B	69/90 (77%)	68 (99%)	1 (1%)	67	86
1	C	69/90 (77%)	69 (100%)	0	100	100
1	D	67/90 (74%)	66 (98%)	1 (2%)	65	85
1	E	32/90 (36%)	31 (97%)	1 (3%)	40	70
1	F	34/90 (38%)	34 (100%)	0	100	100
1	G	80/90 (89%)	80 (100%)	0	100	100
1	H	64/90 (71%)	63 (98%)	1 (2%)	62	84
1	I	73/90 (81%)	72 (99%)	1 (1%)	67	86
1	J	62/90 (69%)	62 (100%)	0	100	100
1	K	29/90 (32%)	27 (93%)	2 (7%)	15	45
1	L	32/90 (36%)	32 (100%)	0	100	100
All	All	676/1080 (63%)	669 (99%)	7 (1%)	76	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	277	ARG
1	D	276	ARG
1	E	288	ASP
1	H	322	MET
1	I	276	ARG
1	K	288	ASP
1	K	341	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	GLN
1	G	289	GLN

5.3.3 RNA ⓘ

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](#)

4 ligands 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	PO4	J	401	-	4,4,4	0.92	0	6,6,6	0.42	0
2	PO4	G	401	-	4,4,4	0.91	0	6,6,6	0.44	0
2	PO4	I	401	-	4,4,4	0.92	0	6,6,6	0.41	0
2	PO4	G	402	-	4,4,4	0.91	0	6,6,6	0.43	0

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 [i](#)

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 [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	106/108 (98%)	-0.13	1 (0%) 84 69	23, 48, 61, 68	0
1	B	106/108 (98%)	-0.16	1 (0%) 84 69	24, 44, 69, 75	0
1	C	107/108 (99%)	-0.20	1 (0%) 84 69	23, 46, 64, 70	0
1	D	107/108 (99%)	-0.17	0 100 100	23, 46, 71, 82	0
1	E	96/108 (88%)	-0.06	2 (2%) 63 43	35, 67, 94, 103	0
1	F	97/108 (89%)	0.04	0 100 100	44, 70, 93, 113	0
1	G	107/108 (99%)	-0.31	0 100 100	25, 42, 55, 69	0
1	H	106/108 (98%)	-0.17	1 (0%) 84 69	24, 46, 59, 75	0
1	I	107/108 (99%)	-0.25	0 100 100	25, 40, 56, 68	0
1	J	106/108 (98%)	-0.17	1 (0%) 84 69	21, 45, 65, 79	0
1	K	96/108 (88%)	0.04	2 (2%) 63 43	35, 69, 91, 97	0
1	L	92/108 (85%)	-0.01	1 (1%) 80 64	39, 68, 88, 91	0
All	All	1233/1296 (95%)	-0.13	10 (0%) 86 72	21, 50, 83, 113	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	309	PRO	3.2
1	K	309	PRO	2.9
1	J	362	THR	2.8
1	K	311	ALA	2.7
1	E	314	PHE	2.3
1	H	295	GLY	2.1
1	C	294	GLN	2.1
1	L	321	GLY	2.1
1	B	295	GLY	2.0
1	A	287	GLY	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](#)

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	PO4	J	401	5/5	0.88	0.51	67,67,92,105	0
2	PO4	G	401	5/5	0.89	0.55	66,71,82,87	0
2	PO4	I	401	5/5	0.91	0.33	62,71,83,93	0
2	PO4	G	402	5/5	0.93	0.46	57,61,81,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.