Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 04:43 AM EDT

PDB ID	:	7N0I
Title	:	Structure of the SARS-CoV-2 N protein C-terminal domain bound to single-domain antibody E2
Authors	:	Ye, Q.; Corbett, K.D.
Deposited on	:	2021-05-25
Resolution	:	2.20 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:

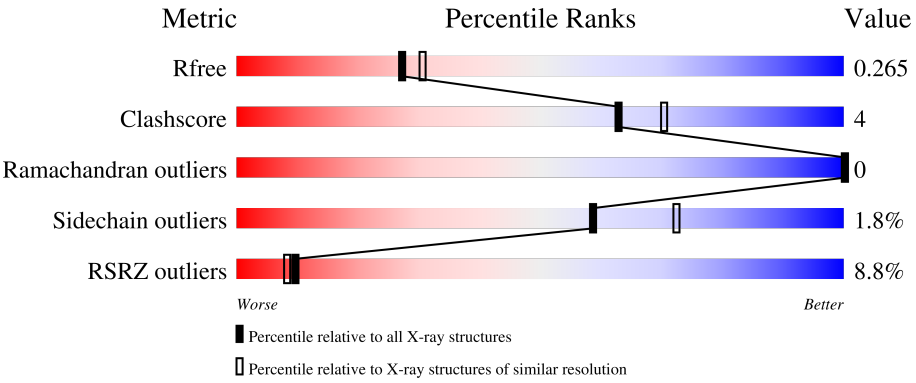
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	96	5% 91% 9%
1	B	96	3% 95% 5%
1	C	96	5% 93% 7%
1	D	96	2% 91% 8%
1	E	96	4% 86% 12%

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Mol	Chain	Length	Quality of chain
1	F	96	22% 85% 14%
1	G	96	27% 90% 10%
1	H	96	42% 83% 15%
2	I	139	3% 91% 6%
2	J	139	87% 9%
2	K	139	84% 9% 6%
2	L	139	87% 7% 6%

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
3	ACT	D	401	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11100 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.

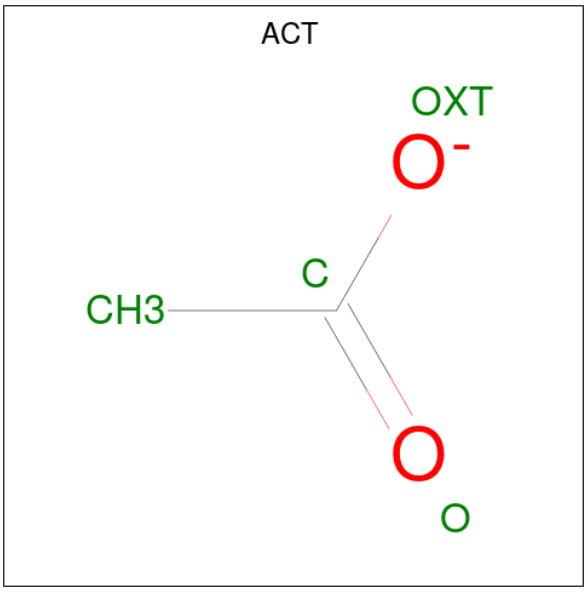
- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	96	Total	C	N	O	S	0	0	0
			765	487	132	144	2			
1	B	96	Total	C	N	O	S	0	0	0
			765	487	132	144	2			
1	C	96	Total	C	N	O	S	0	0	0
			765	487	132	144	2			
1	D	96	Total	C	N	O	S	0	0	0
			765	487	132	144	2			
1	E	96	Total	C	N	O	S	0	0	0
			765	487	132	144	2			
1	F	96	Total	C	N	O	S	0	0	0
			765	487	132	144	2			
1	H	96	Total	C	N	O	S	0	0	0
			765	487	132	144	2			
1	G	96	Total	C	N	O	S	0	0	0
			765	487	132	144	2			

- Molecule 2 is a protein called Single-domain antibody E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	136	Total	C	N	O	S	0	0	0
			1048	650	189	205	4			
2	J	135	Total	C	N	O	S	0	0	0
			1048	650	190	204	4			
2	K	130	Total	C	N	O	S	0	0	0
			1004	623	179	197	5			
2	L	131	Total	C	N	O	S	0	0	0
			1009	626	180	198	5			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	51	Total O 51 51	0	0
5	B	80	Total O 80 80	0	0
5	C	87	Total O 87 87	0	0
5	D	80	Total O 80 80	0	0
5	E	26	Total O 26 26	0	0
5	F	21	Total O 21 21	0	0

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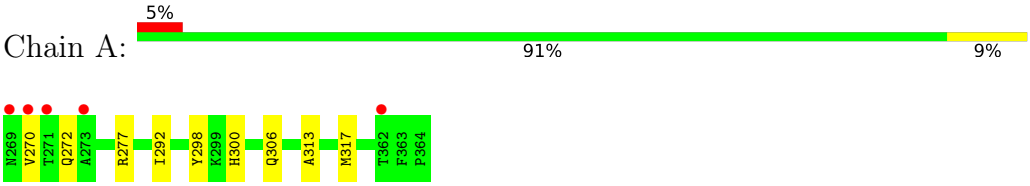
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	17	Total O 17 17	0	0
5	I	97	Total O 97 97	0	0
5	J	125	Total O 125 125	0	0
5	K	123	Total O 123 123	0	0
5	L	135	Total O 135 135	0	0
5	G	20	Total O 20 20	0	0

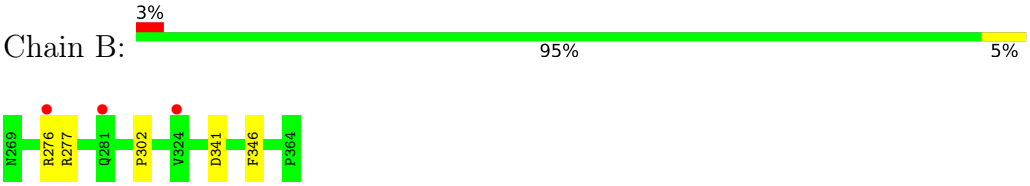
3 Residue-property plots (i)

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.

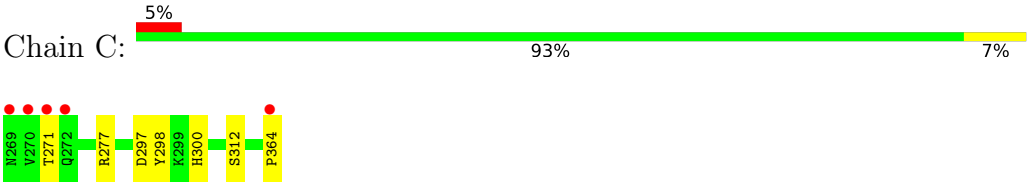
• Molecule 1: Nucleoprotein



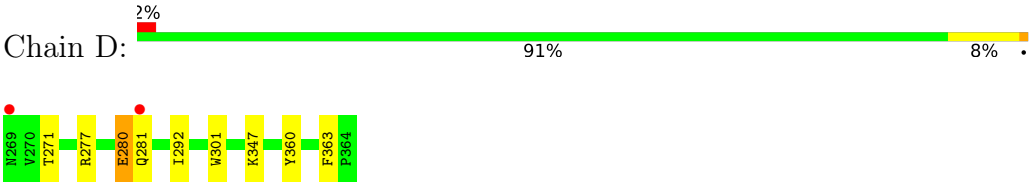
• Molecule 1: Nucleoprotein



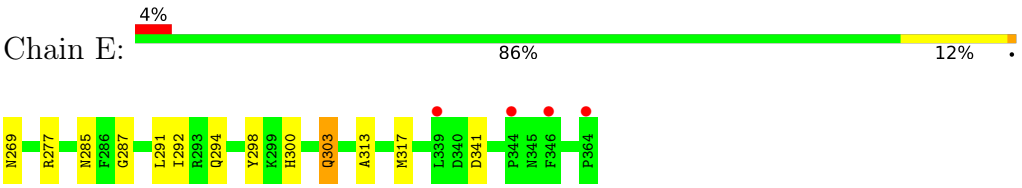
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein

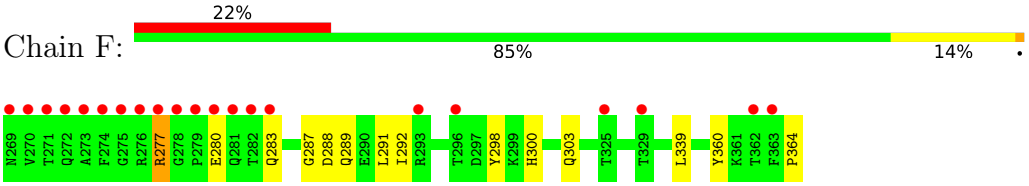


• Molecule 1: Nucleoprotein



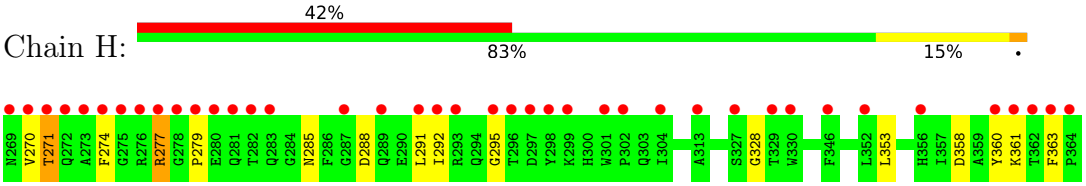
• Molecule 1: Nucleoprotein

Chain F:



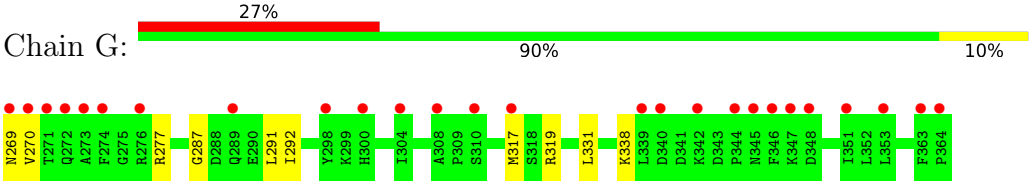
• Molecule 1: Nucleoprotein

Chain H:



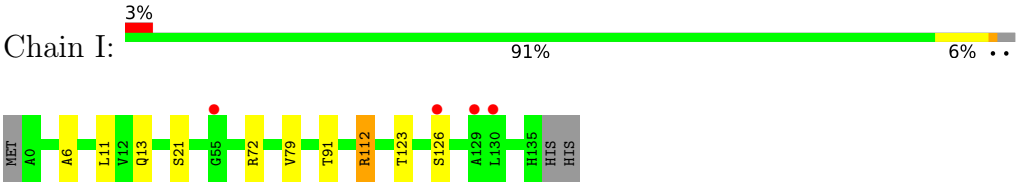
• Molecule 1: Nucleoprotein

Chain G:



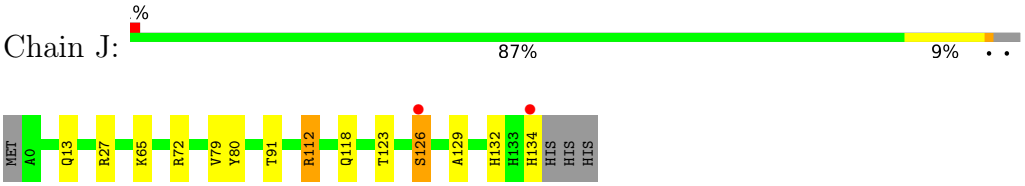
• Molecule 2: Single-domain antibody E2

Chain I:



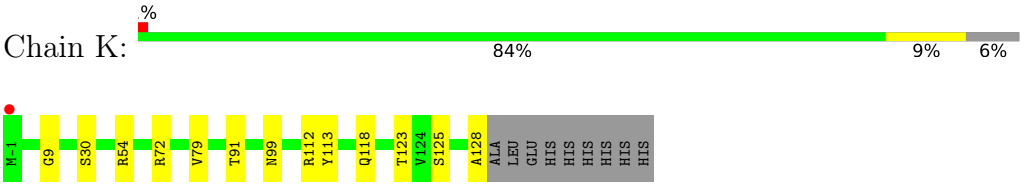
• Molecule 2: Single-domain antibody E2

Chain J:



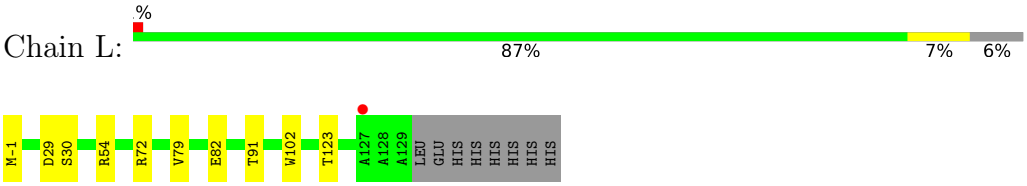
• Molecule 2: Single-domain antibody E2

Chain K:



• Molecule 2: Single-domain antibody E2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.85Å 131.56Å 140.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 2.20 49.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.1 (49.69-2.20) 99.7 (49.69-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.239 , 0.271 0.236 , 0.265	Depositor DCC
R_{free} test set	6589 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11100	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5895e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, MG

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	0.26	0/786	0.50	0/1063
1	B	0.26	0/786	0.50	0/1063
1	C	0.27	0/786	0.49	0/1063
1	D	0.28	0/786	0.51	0/1063
1	E	0.30	0/786	0.49	0/1063
1	F	0.28	0/786	0.49	0/1063
1	G	0.28	0/786	0.52	0/1063
1	H	0.28	0/786	0.51	0/1063
2	I	0.25	0/1073	0.53	0/1458
2	J	0.26	0/1074	0.55	0/1459
2	K	0.27	0/1027	0.57	0/1394
2	L	0.26	0/1032	0.56	0/1401
All	All	0.27	0/10494	0.52	0/14216

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	765	0	733	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	765	0	733	3	0
1	C	765	0	733	4	0
1	D	765	0	733	5	0
1	E	765	0	733	11	0
1	F	765	0	733	9	0
1	G	765	0	733	7	0
1	H	765	0	733	16	0
2	I	1048	0	984	7	0
2	J	1048	0	987	10	0
2	K	1004	0	953	9	0
2	L	1009	0	958	7	0
3	D	4	0	3	2	0
3	G	4	0	3	0	0
4	D	1	0	0	0	0
5	A	51	0	0	1	0
5	B	80	0	0	0	0
5	C	87	0	0	2	0
5	D	80	0	0	3	0
5	E	26	0	0	2	0
5	F	21	0	0	1	0
5	G	20	0	0	0	0
5	H	17	0	0	0	0
5	I	97	0	0	2	0
5	J	125	0	0	2	0
5	K	123	0	0	2	0
5	L	135	0	0	3	0
All	All	11100	0	9752	86	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 4.

All (86) 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:H:270:VAL:HG21	1:H:295:GLY:HA3	1.64	0.79
1:H:358:ASP:HB3	1:H:361:LYS:HE3	1.68	0.75
1:H:328:GLY:HA3	1:G:338:LYS:HE3	1.70	0.74
1:B:276:ARG:HH22	1:D:347:LYS:H	1.40	0.70
1:E:341:ASP:OD2	5:E:401:HOH:O	2.10	0.69
1:E:300:HIS:ND1	1:E:303:GLN:OE1	2.26	0.68
1:E:285:ASN:ND2	5:E:402:HOH:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:72:ARG:HB2	2:L:79:VAL:HG22	1.77	0.67
1:F:277:ARG:HB3	1:F:360:TYR:HB3	1.78	0.66
2:I:72:ARG:HB2	2:I:79:VAL:HG22	1.78	0.66
1:F:339:LEU:O	5:F:401:HOH:O	2.14	0.66
1:C:297:ASP:OD2	5:C:401:HOH:O	2.14	0.65
1:H:288:ASP:HA	1:H:363:PHE:HZ	1.62	0.65
2:J:72:ARG:HB2	2:J:79:VAL:HG22	1.79	0.64
2:J:65:LYS:NZ	5:J:202:HOH:O	2.26	0.64
2:J:129:ALA:HA	2:J:132:HIS:HD2	1.62	0.64
1:G:269:ASN:HB2	1:G:292:ILE:O	1.98	0.64
2:L:30:SER:OG	5:L:201:HOH:O	2.16	0.62
2:K:30:SER:OG	5:K:201:HOH:O	2.14	0.62
2:K:72:ARG:HB2	2:K:79:VAL:HG22	1.81	0.61
1:F:280:GLU:HB2	1:F:283:GLN:HB2	1.84	0.58
2:L:29:ASP:O	2:L:54:ARG:NH2	2.37	0.58
1:H:271:THR:HB	1:H:292:ILE:HG23	1.87	0.57
1:E:313:ALA:O	1:E:317:MET:HG2	2.05	0.56
2:J:129:ALA:HA	2:J:132:HIS:CD2	2.41	0.56
1:F:289:GLN:NE2	1:F:364:PRO:HD2	2.21	0.54
1:E:303:GLN:HE21	1:E:303:GLN:H	1.57	0.51
1:A:272:GLN:O	5:A:401:HOH:O	2.19	0.50
1:C:364:PRO:HD3	5:C:404:HOH:O	2.10	0.50
1:D:360:TYR:HA	1:D:363:PHE:CD2	2.46	0.50
1:F:289:GLN:HE22	1:F:364:PRO:HD2	1.75	0.50
1:A:270:VAL:HB	1:A:292:ILE:HA	1.94	0.50
1:E:303:GLN:HE21	1:E:303:GLN:N	2.10	0.49
2:L:91:THR:HG23	2:L:123:THR:HA	1.93	0.49
2:I:13:GLN:NE2	5:I:205:HOH:O	2.44	0.49
1:A:313:ALA:O	1:A:317:MET:HG2	2.13	0.49
2:I:112:ARG:HH11	2:I:112:ARG:HA	1.78	0.49
1:F:298:TYR:CE2	1:F:300:HIS:HB2	2.48	0.49
1:G:287:GLY:HA2	1:G:291:LEU:HD23	1.95	0.48
1:A:306:GLN:HE22	2:K:118:GLN:HE21	1.61	0.48
2:I:91:THR:HG23	2:I:123:THR:HA	1.95	0.48
2:I:126:SER:HA	5:I:239:HOH:O	2.14	0.47
2:K:54:ARG:HA	2:K:54:ARG:HD3	1.63	0.47
1:A:298:TYR:CE2	1:A:300:HIS:HB2	2.49	0.47
5:D:501:HOH:O	1:H:361:LYS:NZ	2.47	0.47
1:H:271:THR:OG1	1:H:292:ILE:HD12	2.14	0.47
2:K:9:GLY:O	5:K:202:HOH:O	2.20	0.47
1:E:287:GLY:HA2	1:E:291:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:SER:HA	3:D:401:ACT:H3	1.97	0.47
2:L:102:TRP:CE3	1:G:319:ARG:HD3	2.49	0.47
1:H:360:TYR:HA	1:H:363:PHE:CD2	2.51	0.46
2:J:13:GLN:HG2	2:J:126:SER:HA	1.97	0.46
1:F:288:ASP:O	1:F:292:ILE:HG12	2.16	0.45
1:H:353:LEU:HD13	1:G:331:LEU:HD13	1.98	0.45
1:D:301:TRP:CZ3	3:D:401:ACT:H2	2.51	0.45
1:H:288:ASP:O	1:H:292:ILE:HG12	2.16	0.45
1:H:270:VAL:HG21	1:H:295:GLY:CA	2.41	0.44
1:C:298:TYR:CE2	1:C:300:HIS:HB2	2.53	0.44
1:E:294:GLN:NE2	1:E:298:TYR:HA	2.32	0.44
2:K:125:SER:HB2	2:K:128:ALA:HB3	1.98	0.44
2:J:91:THR:HG23	2:J:123:THR:HA	2.00	0.43
2:K:99:ASN:HB3	2:K:113:TYR:HA	1.99	0.43
1:H:277:ARG:HD2	1:H:292:ILE:HD11	1.99	0.43
1:B:302:PRO:HB3	2:K:112:ARG:CZ	2.48	0.43
2:J:112:ARG:NH1	2:J:112:ARG:HA	2.34	0.43
5:D:503:HOH:O	1:H:279:PRO:HG3	2.19	0.42
2:J:27:ARG:HD2	2:J:27:ARG:HA	1.85	0.42
1:D:271:THR:HG23	1:D:292:ILE:HG23	2.01	0.42
1:H:274:PHE:HB3	1:G:317:MET:HG2	2.01	0.42
1:B:341:ASP:HA	1:B:346:PHE:CG	2.55	0.42
1:D:280:GLU:HG3	5:D:535:HOH:O	2.18	0.42
1:E:294:GLN:HE21	1:E:298:TYR:HA	1.83	0.42
1:G:270:VAL:HB	1:G:292:ILE:HA	2.01	0.42
1:F:287:GLY:HA2	1:F:291:LEU:HD23	2.00	0.42
2:I:11:LEU:HG	2:I:123:THR:HB	2.01	0.42
2:K:91:THR:HG23	2:K:123:THR:HA	2.00	0.42
2:L:82:GLU:HB2	5:L:300:HOH:O	2.20	0.41
1:F:303:GLN:OE1	1:F:303:GLN:N	2.52	0.41
1:H:291:LEU:HD12	1:H:295:GLY:HA2	2.02	0.41
1:E:341:ASP:OD1	1:E:341:ASP:N	2.53	0.41
1:H:285:ASN:HB2	1:H:360:TYR:HE2	1.86	0.41
2:J:80:TYR:OH	5:J:201:HOH:O	2.21	0.41
2:L:82:GLU:HG3	5:L:303:HOH:O	2.21	0.41
2:J:112:ARG:HA	2:J:112:ARG:HH11	1.85	0.41
1:E:269:ASN:HB2	1:E:292:ILE:O	2.21	0.40
2:I:6:ALA:HA	2:I:21:SER:O	2.21	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	94/96 (98%)	94 (100%)	0	0	100	100
1	B	94/96 (98%)	94 (100%)	0	0	100	100
1	C	94/96 (98%)	94 (100%)	0	0	100	100
1	D	94/96 (98%)	94 (100%)	0	0	100	100
1	E	94/96 (98%)	94 (100%)	0	0	100	100
1	F	94/96 (98%)	94 (100%)	0	0	100	100
1	G	94/96 (98%)	94 (100%)	0	0	100	100
1	H	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
2	I	134/139 (96%)	133 (99%)	1 (1%)	0	100	100
2	J	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
2	K	128/139 (92%)	127 (99%)	1 (1%)	0	100	100
2	L	129/139 (93%)	128 (99%)	1 (1%)	0	100	100
All	All	1276/1324 (96%)	1271 (100%)	5 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	80/80 (100%)	79 (99%)	1 (1%)	69	81
1	B	80/80 (100%)	79 (99%)	1 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	80/80 (100%)	78 (98%)	2 (2%)	47 60
1	D	80/80 (100%)	77 (96%)	3 (4%)	33 42
1	E	80/80 (100%)	78 (98%)	2 (2%)	47 60
1	F	80/80 (100%)	79 (99%)	1 (1%)	69 81
1	G	80/80 (100%)	79 (99%)	1 (1%)	69 81
1	H	80/80 (100%)	78 (98%)	2 (2%)	47 60
2	I	107/112 (96%)	106 (99%)	1 (1%)	78 88
2	J	108/112 (96%)	104 (96%)	4 (4%)	34 43
2	K	104/112 (93%)	104 (100%)	0	100 100
2	L	104/112 (93%)	103 (99%)	1 (1%)	76 86
All	All	1063/1088 (98%)	1044 (98%)	19 (2%)	59 72

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	ARG
1	B	277	ARG
1	C	271	THR
1	C	277	ARG
1	D	277	ARG
1	D	280	GLU
1	D	281	GLN
1	E	277	ARG
1	E	303	GLN
1	F	277	ARG
1	H	271	THR
1	H	277	ARG
2	I	112	ARG
2	J	112	ARG
2	J	118	GLN
2	J	126	SER
2	J	134	HIS
2	L	-1	MET
1	G	277	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	A	306	GLN
1	A	345	ASN
1	B	272	GLN
1	B	283	GLN
1	B	300	HIS
1	B	306	GLN
1	C	272	GLN
1	D	281	GLN
1	D	306	GLN
1	E	272	GLN
1	E	294	GLN
1	F	272	GLN
1	F	306	GLN
1	F	354	ASN
1	H	272	GLN
1	H	306	GLN
2	I	32	GLN
2	I	132	HIS
2	J	5	GLN
2	J	13	GLN
2	J	32	GLN
2	J	33	HIS
2	J	77	ASN
2	J	118	GLN
2	J	132	HIS
2	J	134	HIS
2	K	33	HIS
2	L	33	HIS
2	L	77	ASN
1	G	272	GLN
1	G	300	HIS
1	G	349	GLN

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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
3	ACT	G	401	-	3,3,3	1.29	0	3,3,3	1.49	0
3	ACT	D	401	-	3,3,3	1.03	0	3,3,3	1.39	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	ACT	2	0

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

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	96/96 (100%)	0.07	5 (5%) 27 26	21, 54, 83, 110	0
1	B	96/96 (100%)	-0.15	3 (3%) 49 47	19, 35, 78, 104	0
1	C	96/96 (100%)	0.08	5 (5%) 27 26	15, 32, 75, 108	0
1	D	96/96 (100%)	0.12	2 (2%) 63 61	13, 31, 78, 105	0
1	E	96/96 (100%)	0.19	4 (4%) 36 34	29, 63, 100, 113	0
1	F	96/96 (100%)	1.43	21 (21%) 0 0	29, 67, 124, 144	0
1	G	96/96 (100%)	1.36	26 (27%) 0 0	40, 88, 126, 145	0
1	H	96/96 (100%)	3.66	40 (41%) 0 0	46, 103, 161, 172	0
2	I	136/139 (97%)	-0.11	4 (2%) 51 49	27, 40, 92, 107	0
2	J	135/139 (97%)	-0.22	2 (1%) 73 72	15, 27, 74, 98	0
2	K	130/139 (93%)	-0.26	1 (0%) 86 85	15, 28, 72, 106	0
2	L	131/139 (94%)	-0.06	1 (0%) 86 85	13, 27, 63, 98	0
All	All	1300/1324 (98%)	0.43	114 (8%) 10 8	13, 42, 111, 172	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	280	GLU	20.4
1	H	270	VAL	19.5
1	H	271	THR	18.7
1	H	281	GLN	17.0
1	H	363	PHE	16.9
1	F	274	PHE	16.1
1	H	278	GLY	15.4
1	H	275	GLY	14.7
1	H	277	ARG	13.4
1	H	274	PHE	13.0
1	H	279	PRO	12.5

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Mol	Chain	Res	Type	RSRZ
1	F	271	THR	10.7
1	H	283	GLN	10.6
1	H	276	ARG	10.3
1	H	362	THR	10.3
1	F	273	ALA	10.0
1	F	280	GLU	9.9
1	H	273	ALA	9.7
1	H	272	GLN	9.7
1	H	296	THR	9.1
1	H	269	ASN	9.0
1	F	276	ARG	8.8
1	G	344	PRO	8.7
1	F	270	VAL	8.6
1	F	275	GLY	8.1
1	F	282	THR	8.0
1	F	363	PHE	7.8
1	G	273	ALA	7.6
1	H	282	THR	7.4
1	G	364	PRO	7.1
1	F	269	ASN	6.6
1	H	361	LYS	6.2
1	A	271	THR	5.8
1	H	292	ILE	5.6
1	C	269	ASN	5.6
1	E	364	PRO	5.6
1	H	291	LEU	5.6
1	H	360	TYR	5.5
1	H	295	GLY	5.3
1	E	346	PHE	4.8
1	F	277	ARG	4.8
1	F	272	GLN	4.7
1	G	346	PHE	4.7
1	A	273	ALA	4.6
1	H	298	TYR	4.5
2	I	126	SER	4.5
1	F	283	GLN	4.1
1	G	317	MET	4.1
1	H	293	ARG	4.0
1	H	327	SER	3.9
1	F	279	PRO	3.9
1	G	339	LEU	3.8
1	H	352	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	278	GLY	3.7
1	H	346	PHE	3.7
1	H	304	ILE	3.6
1	G	310	SER	3.5
1	H	297	ASP	3.4
1	G	351	ILE	3.4
1	D	269	ASN	3.4
1	G	271	THR	3.4
1	B	276	ARG	3.3
1	A	269	ASN	3.3
1	E	344	PRO	3.2
1	F	281	GLN	3.2
1	C	272	GLN	3.1
1	G	274	PHE	3.1
2	I	129	ALA	3.1
2	L	127	ALA	3.1
1	G	304	ILE	3.1
1	G	276	ARG	3.1
1	G	340	ASP	3.1
1	C	364	PRO	2.9
1	G	342	LYS	2.9
1	A	270	VAL	2.9
1	G	272	GLN	2.9
1	F	362	THR	2.9
2	I	130	LEU	2.9
1	G	300	HIS	2.9
2	K	-1	MET	2.8
1	F	329	THR	2.8
1	G	269	ASN	2.7
1	G	270	VAL	2.7
1	C	271	THR	2.7
1	G	363	PHE	2.7
1	F	296	THR	2.6
2	J	134	HIS	2.6
1	G	289	GLN	2.6
1	G	347	LYS	2.6
1	E	339	LEU	2.5
1	B	281	GLN	2.5
1	G	353	LEU	2.5
1	A	362	THR	2.5
1	H	330	TRP	2.5
1	H	289	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	287	GLY	2.4
2	I	55	GLY	2.4
1	G	298	TYR	2.4
1	H	301	TRP	2.4
1	H	356	HIS	2.4
1	G	308	ALA	2.4
1	D	281	GLN	2.4
1	G	345	ASN	2.3
1	G	348	ASP	2.3
1	F	325	THR	2.3
1	H	302	PRO	2.2
1	B	324	VAL	2.2
1	H	329	THR	2.2
1	C	270	VAL	2.1
1	H	364	PRO	2.1
1	H	299	LYS	2.1
1	H	313	ALA	2.0
2	J	126	SER	2.0
1	F	293	ARG	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, 95^{th} 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
4	MG	D	402	1/1	0.88	0.09	31,31,31,31	0
3	ACT	G	401	4/4	0.90	0.17	67,69,70,72	0
3	ACT	D	401	4/4	0.93	0.29	39,39,40,51	0

6.5 Other polymers (i)

There are no such residues in this entry.