



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2016 – 04:53 AM EST

PDB ID : 5KQ4
Title : Crystal structure of *S. pombe* Dcp1/Dcp2 in complex with *H. sapiens* PNRC2 and synthetic cap analog
Authors : Mugridge, J.S.; Ziemniak, M.; Jemielity, J.; Gross, J.D.
Deposited on : 2016-07-05
Resolution : 2.56 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

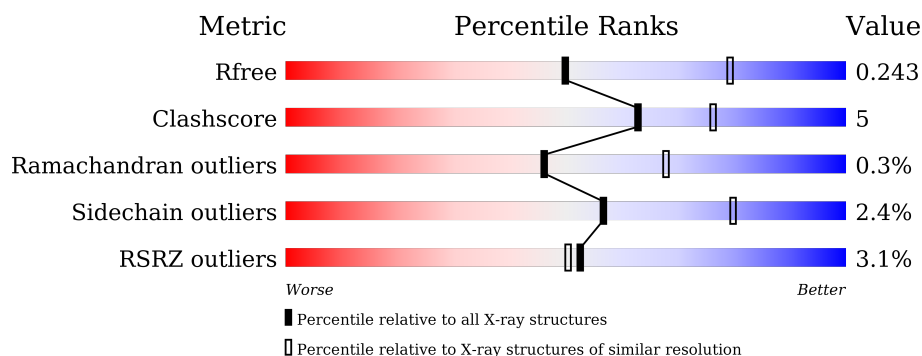
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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}	91344	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	130	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div> </div>
1	D	130	<div> <div></div> <div> <div>87%</div> <div>10%</div> <div>•</div> </div> </div>
2	C	31	<div> <div>3%</div> <div> <div></div> <div>48%</div> <div>26%</div> <div>26%</div> </div> </div>
2	F	31	<div> <div></div> <div> <div>71%</div> <div>29%</div> </div> </div>
3	B	249	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>•</div> </div> </div>
3	E	249	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>6%</div> </div> </div>

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
4	6VQ	E	301	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6488 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 mRNA-decapping enzyme subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	126	Total	C	N	O	S	0	0	0
			1048	675	182	188	3			
1	A	124	Total	C	N	O	S	0	0	0
			1032	663	180	186	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP Q9P805
D	-1	GLU	-	expression tag	UNP Q9P805
D	0	PHE	-	expression tag	UNP Q9P805
A	-2	GLY	-	expression tag	UNP Q9P805
A	-1	GLU	-	expression tag	UNP Q9P805
A	0	PHE	-	expression tag	UNP Q9P805

- Molecule 2 is a protein called Proline-rich nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	22	Total	C	N	O	0	0	0
			170	114	27	29			
2	C	23	Total	C	N	O	0	0	0
			176	117	28	31			

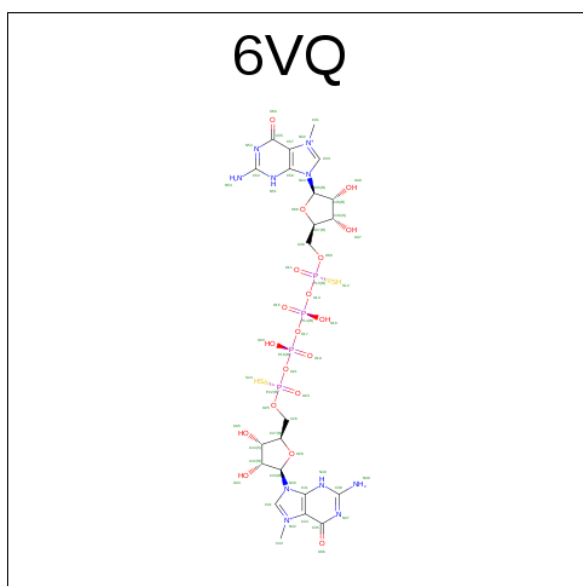
- Molecule 3 is a protein called mRNA decapping complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	235	Total	C	N	O	S	0	0	0
			1934	1246	330	346	12			
3	B	242	Total	C	N	O	S	0	0	0
			1987	1278	342	354	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	GLY	-	expression tag	UNP O13828
E	-3	GLY	-	expression tag	UNP O13828
E	-2	GLY	-	expression tag	UNP O13828
E	-1	GLY	-	expression tag	UNP O13828
E	0	SER	-	expression tag	UNP O13828
B	-4	GLY	-	expression tag	UNP O13828
B	-3	GLY	-	expression tag	UNP O13828
B	-2	GLY	-	expression tag	UNP O13828
B	-1	GLY	-	expression tag	UNP O13828
B	0	SER	-	expression tag	UNP O13828

- Molecule 4 is $[[(2 \{R\}, 3 \{S\}, 4 \{R\}, 5 \{R\}) - 5 - (2\text{-azanyl-7-methyl-6-oxidanylidene-3 \{H\}-purin-7-ium-9-yl}) - 3,4\text{-bis(oxidanyl)oxolan-2-yl}] \text{methoxy-sulfanyl-phosphoryl}] [[(2 \{R\}, 3 \{S\}, 4 \{R\}, 5 \{R\}) - 5 - (2\text{-azanyl-7-methyl-6-oxidanylidene-3 \{H\}-purin-7-ium-9-yl}) - 3,4\text{-bis(oxidanyl)oxolan-2-yl}] \text{methoxy-sulfanyl-phosphoryl}] \text{oxy-oxidanyl-phosphoryl}] \text{hydrogen phosphate}$ (three-letter code: 6VQ) (formula: $\text{C}_{22}\text{H}_{34}\text{N}_{10}\text{O}_{19}\text{P}_4\text{S}_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	S	0	0
			57	22	10	19	4	2		
4	B	1	Total	C	N	O	P	S	0	0
			57	22	10	19	4	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	O	0	0
			2	2		

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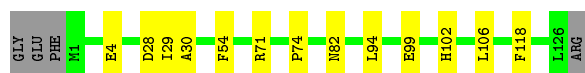
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total 1	O 1	0	0
5	E	14	Total 14	O 14	0	0
5	A	1	Total 1	O 1	0	0
5	B	9	Total 9	O 9	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

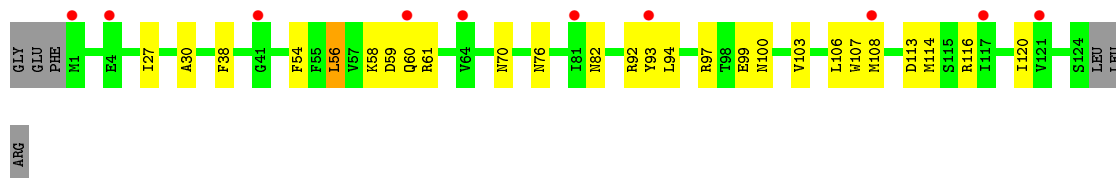
- Molecule 1: mRNA-decapping enzyme subunit 1

Chain D: 



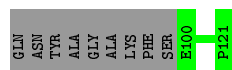
- Molecule 1: mRNA-decapping enzyme subunit 1

Chain A: 



- Molecule 2: Proline-rich nuclear receptor coactivator 2

Chain F: 




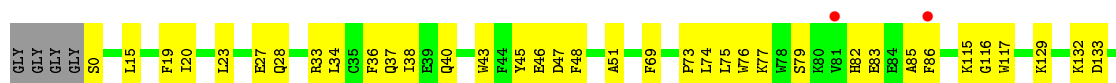
- Molecule 2: Proline-rich nuclear receptor coactivator 2

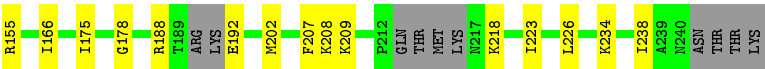
Chain C: 



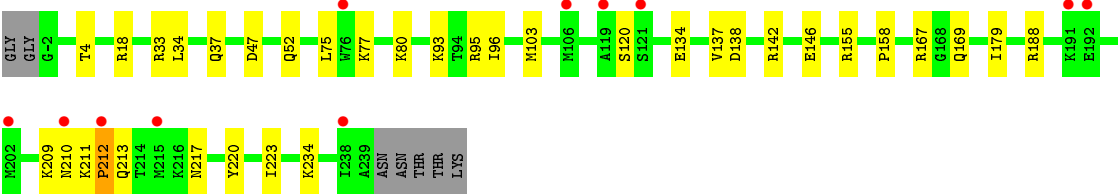
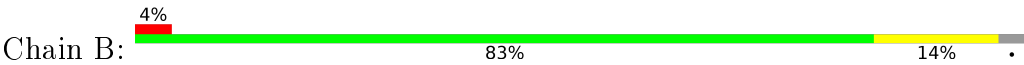
- Molecule 3: mRNA decapping complex subunit 2

Chain E: 





• Molecule 3: mRNA decapping complex subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.07Å 120.75Å 91.85Å 90.00° 97.90° 90.00°	Depositor
Resolution (Å)	45.49 – 2.56 45.49 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.49-2.56) 92.3 (45.49-2.56)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.87 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.206 , 0.251 0.200 , 0.243	Depositor DCC
R_{free} test set	1355 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.0	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	0.94	EDS
Total number of atoms	6488	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: 6VQ

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	0/1057	0.52	0/1434
1	D	0.28	0/1073	0.50	0/1456
2	C	0.29	0/187	0.48	0/262
2	F	0.29	0/181	0.44	0/254
3	B	0.30	1/2037 (0.0%)	0.43	0/2745
3	E	0.27	0/1982	0.42	0/2672
All	All	0.28	1/6517 (0.0%)	0.46	0/8823

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	120	SER	CA-CB	6.25	1.62	1.52

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	1032	0	1017	17	1
1	D	1048	0	1039	9	0
2	C	176	0	169	4	0
2	F	170	0	164	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1987	0	1985	18	0
3	E	1934	0	1920	26	1
4	B	57	0	0	0	0
4	E	57	0	0	0	0
5	A	1	0	0	1	0
5	B	9	0	0	0	0
5	D	2	0	0	0	0
5	E	14	0	0	2	0
5	F	1	0	0	0	0
All	All	6488	0	6294	68	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 5.

All (68) 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)
3:E:175:ILE:O	5:E:401:HOH:O	2.01	0.78
1:A:30:ALA:HB3	1:A:54:PHE:HB3	1.66	0.77
1:D:30:ALA:HB3	1:D:54:PHE:HB3	1.74	0.69
1:A:59:ASP:OD1	1:A:60:GLN:N	2.31	0.64
1:D:71:ARG:NH2	3:E:37:GLN:OE1	2.28	0.62
3:E:79:SER:HB2	3:E:83:GLU:HA	1.82	0.61
3:E:20:ILE:HG21	3:E:75:LEU:HD11	1.84	0.60
3:B:93:LYS:HB3	3:B:169:GLN:HB2	1.83	0.59
3:B:4:THR:HG22	3:B:52:GLN:HB3	1.85	0.58
1:D:4:GLU:HB3	3:E:74:LEU:HD21	1.85	0.57
3:E:23:LEU:HD11	3:E:37:GLN:HG3	1.88	0.56
3:B:210:ASN:O	3:B:212:PRO:HD3	2.05	0.56
1:A:27:ILE:HD11	1:A:58:LYS:HG3	1.88	0.55
1:D:94:LEU:HB2	1:D:106:LEU:HB2	1.90	0.54
1:A:100:ASN:O	5:A:201:HOH:O	2.18	0.54
3:E:38:ILE:HD12	3:E:86:PHE:CE1	2.44	0.53
3:B:103:MET:HB3	3:B:179:ILE:HD12	1.91	0.52
1:A:113:ASP:OD1	1:A:116:ARG:NH1	2.43	0.52
3:B:47:ASP:HB3	3:B:217:ASN:HB3	1.91	0.51
3:B:93:LYS:HD2	3:B:167:ARG:HD3	1.91	0.51
1:A:70:ASN:O	3:B:18:ARG:NE	2.42	0.51
1:A:116:ARG:O	1:A:120:ILE:HG13	2.12	0.50
1:A:82:ASN:OD1	1:A:99:GLU:HG2	2.12	0.50
1:A:27:ILE:HD12	1:A:56:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASN:OD1	3:B:18:ARG:NH2	2.46	0.49
1:A:92:ARG:NH2	1:A:108:MET:O	2.44	0.48
3:B:142:ARG:O	3:B:146:GLU:HG3	2.13	0.48
1:D:94:LEU:HD21	1:D:118:PHE:HB2	1.96	0.48
1:A:108:MET:HG3	1:A:114:MET:HA	1.95	0.48
3:B:95:ARG:HG2	3:B:96:ILE:HG13	1.96	0.47
2:C:100:GLU:HB3	2:C:101:PRO:HD2	1.96	0.47
1:D:74:PRO:HG3	3:E:48:PHE:HB3	1.97	0.47
3:B:137:VAL:HG21	3:B:158:PRO:HG3	1.98	0.46
1:D:82:ASN:HD22	1:D:99:GLU:HG2	1.80	0.46
3:E:27:GLU:HG3	3:E:33:ARG:HG2	1.97	0.45
3:B:33:ARG:O	3:B:37:GLN:HG2	2.17	0.45
3:E:46:GLU:OE1	5:E:402:HOH:O	2.21	0.45
3:E:43:TRP:HA	3:E:166:ILE:HD11	1.98	0.45
3:E:155:ARG:NH1	3:E:178:GLY:O	2.49	0.44
3:E:117:TRP:HE1	3:E:192:GLU:N	2.16	0.44
3:E:36:PHE:O	3:E:40:GLN:HG2	2.17	0.44
3:E:207:PHE:HB2	3:E:226:LEU:HD13	1.99	0.44
3:E:202:MET:HG2	3:E:208:LYS:HE3	1.98	0.44
3:E:234:LYS:HZ2	3:E:238:ILE:HD11	1.83	0.44
3:E:15:LEU:HD11	3:E:45:TYR:HB2	2.00	0.44
3:E:234:LYS:NZ	3:E:238:ILE:HD11	2.33	0.43
1:A:94:LEU:HB2	1:A:106:LEU:HB2	2.01	0.43
3:B:234:LYS:HE3	3:B:234:LYS:HB2	1.84	0.43
1:D:102:HIS:CD2	2:C:119:PHE:HA	2.54	0.42
3:E:51:ALA:HB2	3:E:223:ILE:HD13	2.01	0.42
3:E:82:HIS:HB3	3:E:85:ALA:HB2	2.01	0.42
3:E:73:PRO:HA	3:E:76:TRP:CE2	2.54	0.42
1:A:92:ARG:NH1	1:A:108:MET:O	2.53	0.41
1:A:38:PHE:HB3	1:A:103:VAL:HG13	2.03	0.41
3:E:132:LYS:O	3:E:133:ASP:HB2	2.20	0.41
3:E:115:LYS:HG2	3:E:116:GLY:O	2.21	0.41
3:B:134:GLU:OE1	3:B:142:ARG:NE	2.43	0.41
3:B:77:LYS:HB2	3:B:77:LYS:HE3	1.80	0.41
3:E:19:PHE:HB2	3:E:20:ILE:HD12	2.02	0.41
1:A:93:TYR:CE1	1:A:107:TRP:HD1	2.39	0.41
1:D:28:ASP:OD1	1:D:29:ILE:N	2.50	0.41
3:B:211:LYS:HB2	3:B:211:LYS:HE3	1.72	0.41
2:C:103:SER:O	2:C:106:VAL:HG22	2.20	0.41
3:B:75:LEU:HA	3:B:75:LEU:HD23	1.86	0.41
3:B:220:TYR:HA	3:B:223:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:120:ASN:HA	2:C:121:PRO:HD2	1.91	0.40
3:E:218:LYS:HA	3:E:218:LYS:HD3	1.55	0.40
1:A:61:ARG:HB3	1:A:61:ARG:HE	1.71	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)
3:E:133:ASP:OD2	1:A:97:ARG:NH2[2_545]	2.12	0.08

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	122/130 (94%)	121 (99%)	1 (1%)	0	100	100
1	D	124/130 (95%)	123 (99%)	1 (1%)	0	100	100
2	C	21/31 (68%)	21 (100%)	0	0	100	100
2	F	20/31 (64%)	20 (100%)	0	0	100	100
3	B	240/249 (96%)	228 (95%)	10 (4%)	2 (1%)	24	43
3	E	229/249 (92%)	222 (97%)	7 (3%)	0	100	100
All	All	756/820 (92%)	735 (97%)	19 (2%)	2 (0%)	46	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	213	GLN
3	B	212	PRO

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	116/121 (96%)	115 (99%)	1 (1%)	84	94
1	D	118/121 (98%)	118 (100%)	0	100	100
2	C	23/28 (82%)	22 (96%)	1 (4%)	35	60
2	F	22/28 (79%)	22 (100%)	0	100	100
3	B	218/223 (98%)	212 (97%)	6 (3%)	51	76
3	E	213/223 (96%)	204 (96%)	9 (4%)	36	61
All	All	710/744 (95%)	693 (98%)	17 (2%)	57	80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	0	SER
3	E	28	GLN
3	E	34	LEU
3	E	47	ASP
3	E	69	PHE
3	E	77	LYS
3	E	129	LYS
3	E	188	ARG
3	E	209	LYS
1	A	56	LEU
2	C	118	SER
3	B	34	LEU
3	B	80	LYS
3	B	138	ASP
3	B	155	ARG
3	B	188	ARG
3	B	209	LYS

Some 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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
4	6VQ	B	301	-	44,62,62	4.04	16 (36%)	52,99,99	2.97	19 (36%)
4	6VQ	E	301	-	44,62,62	4.19	17 (38%)	52,99,99	2.79	18 (34%)

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
4	6VQ	B	301	-	-	0/20/70/70	0/6/6/6
4	6VQ	E	301	-	-	0/20/70/70	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	6VQ	O09-C08	-2.67	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	301	6VQ	O09-C08	-2.39	1.35	1.44
4	B	301	6VQ	O25-C26	-2.12	1.36	1.44
4	E	301	6VQ	C41-N40	2.17	1.39	1.35
4	E	301	6VQ	C44-C27	2.29	1.59	1.53
4	B	301	6VQ	C08-C07	2.41	1.59	1.51
4	E	301	6VQ	C08-C07	2.47	1.59	1.51
4	B	301	6VQ	C35-C34	3.05	1.47	1.41
4	B	301	6VQ	C26-C27	3.19	1.62	1.51
4	E	301	6VQ	C55-C57	3.21	1.47	1.41
4	E	301	6VQ	C31-N32	3.23	1.39	1.33
4	B	301	6VQ	C55-C57	3.30	1.48	1.41
4	B	301	6VQ	C31-N32	3.31	1.39	1.33
4	B	301	6VQ	C03-N02	3.32	1.39	1.33
4	B	301	6VQ	C31-N30	3.45	1.39	1.33
4	E	301	6VQ	C35-C34	3.47	1.48	1.41
4	E	301	6VQ	C03-N02	3.49	1.39	1.33
4	E	301	6VQ	C26-C27	3.56	1.63	1.51
4	E	301	6VQ	C31-N30	3.58	1.39	1.33
4	B	301	6VQ	C52-N53	3.88	1.42	1.34
4	E	301	6VQ	C52-N53	3.94	1.42	1.34
4	E	301	6VQ	C38-N39	4.38	1.43	1.34
4	B	301	6VQ	C38-N39	4.45	1.43	1.34
4	B	301	6VQ	C03-N04	4.97	1.42	1.33
4	E	301	6VQ	C03-N04	5.05	1.42	1.33
4	E	301	6VQ	C35-N37	5.08	1.42	1.33
4	B	301	6VQ	C35-N37	5.23	1.42	1.33
4	B	301	6VQ	C55-N54	5.28	1.42	1.33
4	E	301	6VQ	C55-N54	5.33	1.42	1.33
4	B	301	6VQ	P10-O09	13.62	1.79	1.58
4	E	301	6VQ	P10-O09	14.65	1.80	1.58
4	B	301	6VQ	P22-O25	17.33	1.85	1.58
4	E	301	6VQ	P22-O25	17.86	1.86	1.58

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	6VQ	C34-C35-N37	-6.22	115.39	123.52
4	E	301	6VQ	C34-C35-N37	-6.06	115.59	123.52
4	B	301	6VQ	C57-C55-N54	-5.66	116.13	123.52
4	E	301	6VQ	C57-C55-N54	-5.63	116.16	123.52
4	B	301	6VQ	C48-C05-N04	-5.03	100.01	113.47
4	E	301	6VQ	C55-C57-C50	-4.86	115.30	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	6VQ	O25-P22-O23	-4.55	97.10	114.14
4	E	301	6VQ	O09-P10-O11	-4.47	97.41	114.14
4	E	301	6VQ	O25-P22-O23	-4.37	97.77	114.14
4	B	301	6VQ	O09-P10-O11	-4.31	98.02	114.14
4	B	301	6VQ	C55-C57-C50	-3.85	116.46	120.86
4	E	301	6VQ	N51-C52-N54	-3.70	122.52	127.56
4	B	301	6VQ	N51-C52-N54	-3.06	123.40	127.56
4	B	301	6VQ	N40-C38-N37	-2.83	123.70	127.56
4	E	301	6VQ	C48-C05-N04	-2.78	106.02	113.47
4	B	301	6VQ	C35-C34-C41	-2.65	117.83	120.86
4	E	301	6VQ	O45-C44-C42	-2.58	103.51	111.86
4	B	301	6VQ	O45-C44-C42	-2.57	103.53	111.86
4	E	301	6VQ	N40-C38-N37	-2.33	124.38	127.56
4	E	301	6VQ	O20-P18-O17	2.06	114.09	105.27
4	E	301	6VQ	O25-C26-C27	2.24	117.16	109.09
4	E	301	6VQ	C42-C44-C27	2.32	107.38	102.64
4	B	301	6VQ	O20-P18-O17	2.37	115.44	105.27
4	B	301	6VQ	C27-O28-C29	2.39	112.17	109.64
4	B	301	6VQ	O21-P22-O25	2.59	111.01	101.46
4	B	301	6VQ	C07-O06-C05	2.88	112.70	109.64
4	E	301	6VQ	O21-P22-O25	3.44	114.15	101.46
4	B	301	6VQ	O28-C29-N30	4.43	116.48	108.11
4	E	301	6VQ	C05-N04-C50	4.44	131.75	126.81
4	E	301	6VQ	O28-C29-N30	4.47	116.54	108.11
4	E	301	6VQ	C35-N37-C38	5.20	121.98	115.88
4	B	301	6VQ	C55-N54-C52	5.55	122.39	115.88
4	B	301	6VQ	C35-N37-C38	5.82	122.70	115.88
4	B	301	6VQ	C05-N04-C50	6.10	133.61	126.81
4	E	301	6VQ	C55-N54-C52	6.26	123.21	115.88
4	E	301	6VQ	O06-C05-N04	8.71	124.56	108.11
4	B	301	6VQ	O06-C05-N04	10.14	127.26	108.11

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	124/130 (95%)	0.53	10 (8%) 15 13	56, 95, 133, 154	0
1	D	126/130 (96%)	0.05	0 100 100	38, 60, 92, 131	0
2	C	23/31 (74%)	0.40	1 (4%) 39 36	98, 113, 122, 126	0
2	F	22/31 (70%)	0.03	0 100 100	47, 64, 105, 127	0
3	B	242/249 (97%)	0.33	11 (4%) 37 34	48, 81, 121, 147	0
3	E	235/249 (94%)	0.07	2 (0%) 85 85	35, 58, 107, 126	0
All	All	772/820 (94%)	0.23	24 (3%) 52 50	35, 75, 121, 154	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	191	LYS	7.8
1	A	41	GLY	3.8
1	A	117	ILE	3.8
3	B	121	SER	3.6
3	E	81	VAL	3.4
3	B	212	PRO	3.3
3	B	215	MET	3.1
3	B	210	ASN	3.1
1	A	1	MET	3.0
1	A	81	ILE	2.9
1	A	64	VAL	2.8
1	A	93	TYR	2.8
1	A	4	GLU	2.7
3	B	238	ILE	2.5
3	B	106	MET	2.5
1	A	108	MET	2.4
3	B	76	TRP	2.4
1	A	60	GLN	2.4
2	C	119	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	121	VAL	2.2
3	E	86	PHE	2.1
3	B	202	MET	2.1
3	B	119	ALA	2.1
3	B	192	GLU	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q < 0.9
4	6VQ	E	301	57/57	0.64	0.26	2.55	123,149,170,173	0
4	6VQ	B	301	57/57	0.93	0.14	-0.56	52,88,105,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.