



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:37 AM EDT

PDB ID : 2F6M / pdb_00002f6m
Title : Structure of a Vps23-C:Vps28-N subcomplex
Authors : Kostelansky, M.S.; Lee, S.; Kim, J.; Hurley, J.H.
Deposited on : 2005-11-29
Resolution : 2.10 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

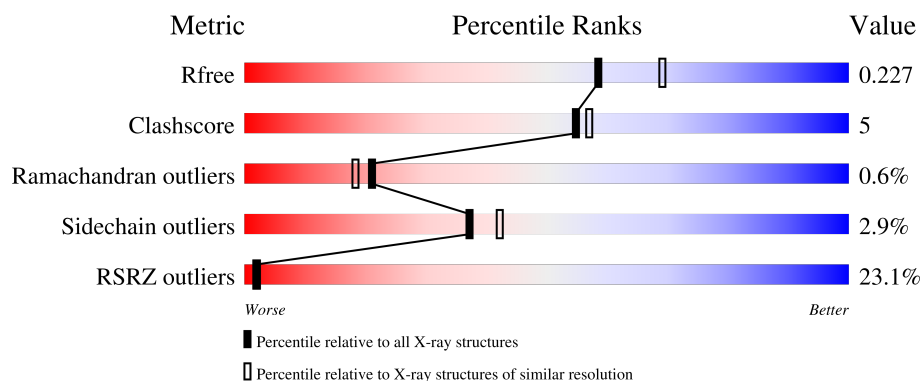
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	65	14% 86% 14%
1	C	65	11% 82% 12% • •
2	B	109	26% 87% 10% • •
2	D	109	31% 80% 13% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2913 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 Suppressor protein STP22 of temperature-sensitive alpha-factor receptor and arginine permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	65	Total	C	N	O	S	0	0	0
			531	335	97	97	2			
1	C	63	Total	C	N	O	S	0	0	0
			516	326	95	93	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	321	MET	-	cloning artifact	UNP P25604
A	344	ALA	CYS	engineered mutation	UNP P25604
C	321	MET	-	cloning artifact	UNP P25604
C	344	ALA	CYS	engineered mutation	UNP P25604

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein VPS28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	107	Total	C	N	O	S	0	0	0
			874	552	140	181	1			
2	D	102	Total	C	N	O		0	0	0
			839	532	135	172				

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLY	-	cloning artifact	UNP Q02767
B	11	ALA	-	cloning artifact	UNP Q02767
B	12	MET	-	cloning artifact	UNP Q02767
B	101	ALA	CYS	engineered mutation	UNP Q02767
D	10	GLY	-	cloning artifact	UNP Q02767
D	11	ALA	-	cloning artifact	UNP Q02767
D	12	MET	-	cloning artifact	UNP Q02767

Continued on next page...

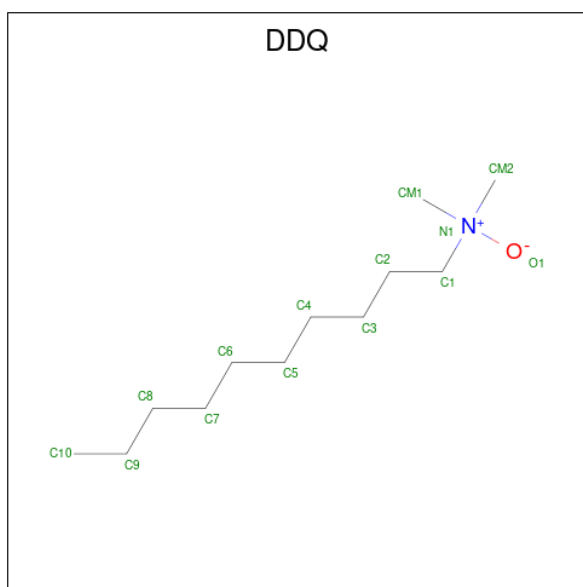
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	101	ALA	CYS	engineered mutation	UNP Q02767

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: C₁₂H₂₇NO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 12 1 1	0	0
4	A	1	Total C N O 14 12 1 1	0	0
4	A	1	Total C N O 14 12 1 1	0	0
4	B	1	Total C N O 14 12 1 1	0	0
4	B	1	Total C N O 14 12 1 1	0	0
4	C	1	Total C N O 14 12 1 1	0	0
4	C	1	Total C N O 14 12 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	12	1	1		

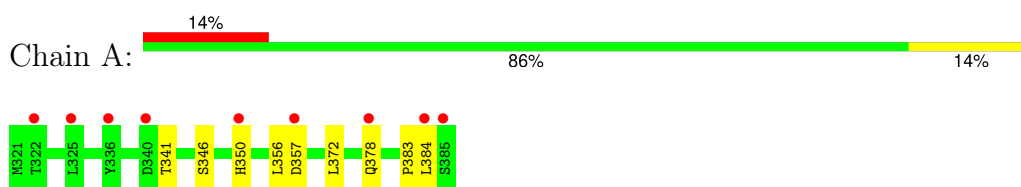
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	9	Total	O	0	0
			9	9		
5	C	16	Total	O	0	0
			16	16		
5	D	4	Total	O	0	0
			4	4		

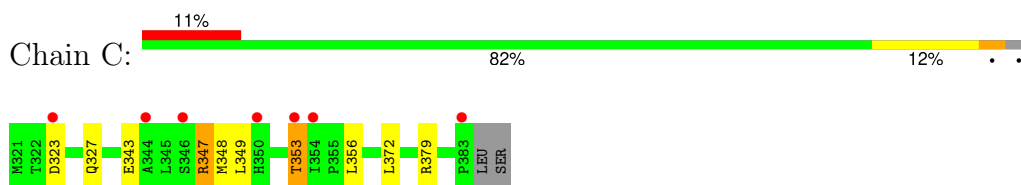
3 Residue-property plots [i](#)

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.

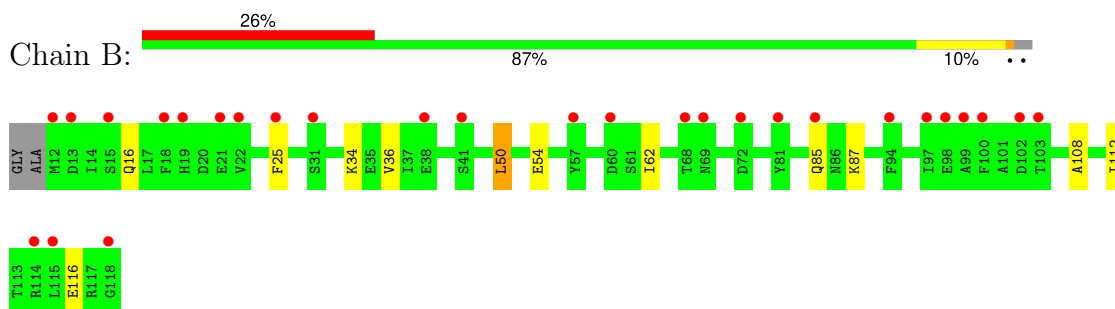
- Molecule 1: Suppressor protein STP22 of temperature-sensitive alpha-factor receptor and arginine permease



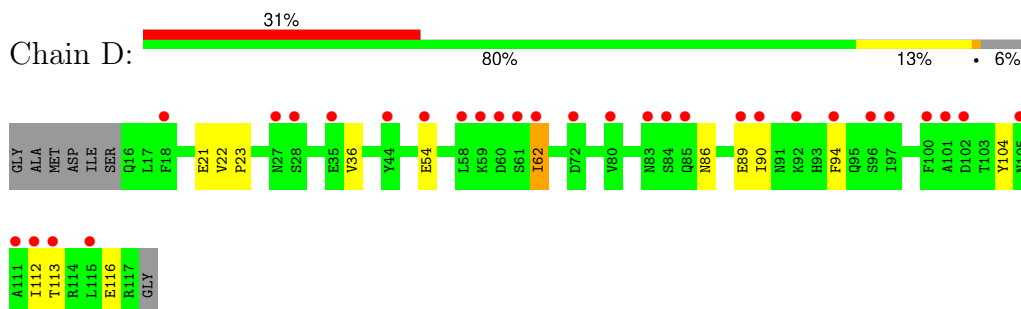
- Molecule 1: Suppressor protein STP22 of temperature-sensitive alpha-factor receptor and arginine permease



- Molecule 2: Vacuolar protein sorting-associated protein VPS28



- Molecule 2: Vacuolar protein sorting-associated protein VPS28



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.24Å 119.25Å 125.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.51 – 2.10 19.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.51-2.10) 97.3 (19.51-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.67 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.241 , 0.261 0.241 , 0.227	Depositor DCC
R_{free} test set	1318 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2913	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 22.40 % 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 5.7495e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: DDQ, 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	0.56	0/540	0.84	0/730
1	C	0.51	0/525	0.86	0/711
2	B	0.45	0/887	0.78	0/1198
2	D	0.49	0/852	0.82	0/1153
All	All	0.50	0/2804	0.82	0/3792

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	531	0	537	7	0
1	C	516	0	521	10	0
2	B	874	0	855	7	0
2	D	839	0	823	10	0
3	A	1	0	0	0	0
4	A	42	0	81	3	0
4	B	28	0	54	1	0
4	C	28	0	54	0	0
4	D	14	0	27	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	11	0	0	0	0
5	B	9	0	0	0	0
5	C	16	0	0	0	0
5	D	4	0	0	0	0
All	All	2913	0	2952	28	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 5.

All (28) 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:327:GLN:HE22	2:D:22:VAL:H	1.22	0.87
1:A:341:THR:HG21	4:A:101:DDQ:CM2	2.06	0.86
1:C:348:MET:HE2	1:C:353:THR:HG22	1.62	0.81
1:C:379:ARG:NH1	2:D:23:PRO:O	2.19	0.76
1:C:349:LEU:HD11	2:D:62:ILE:HD11	1.72	0.71
2:B:112:ILE:O	2:B:116:GLU:HG2	1.95	0.67
1:A:378:GLN:HG2	4:B:119:DDQ:H42	1.78	0.66
1:A:341:THR:HG21	4:A:101:DDQ:HM22	1.78	0.65
1:C:356:LEU:HD22	2:D:62:ILE:HG12	1.79	0.64
1:C:348:MET:HE2	1:C:353:THR:CG2	2.29	0.63
2:D:86:ASN:HB3	2:D:89:GLU:HB2	1.82	0.61
1:C:323:ASP:HB3	2:D:21:GLU:HG3	1.87	0.55
1:A:341:THR:HG21	4:A:101:DDQ:HM23	1.92	0.51
1:A:346:SER:O	1:A:350:HIS:CD2	2.64	0.50
2:D:108:ALA:O	2:D:112:ILE:HG12	2.13	0.49
1:C:348:MET:CE	1:C:353:THR:CG2	2.91	0.49
1:C:343:GLU:O	1:C:347:ARG:HG2	2.12	0.48
2:B:36:VAL:HG22	2:B:85:GLN:HB3	1.96	0.48
1:A:346:SER:O	1:A:350:HIS:HD2	1.96	0.47
2:B:85:GLN:C	2:B:87:LYS:H	2.23	0.46
1:A:356:LEU:HD22	2:B:62:ILE:HG21	1.99	0.44
2:D:94:PHE:HE1	2:D:104:TYR:HE1	1.66	0.43
2:B:108:ALA:O	2:B:112:ILE:HG12	2.19	0.43
1:C:343:GLU:OE2	1:C:347:ARG:HD3	2.20	0.42
2:D:36:VAL:HG13	2:D:90:ILE:HG22	2.02	0.41
2:D:113:THR:O	2:D:116:GLU:HG2	2.19	0.41
2:B:25:PHE:CE1	2:B:34:LYS:HE3	2.55	0.41
2:B:50:LEU:HD22	2:B:54:GLU:HG2	2.02	0.41

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	63/65 (97%)	61 (97%)	0	2 (3%)	3	1
1	C	61/65 (94%)	61 (100%)	0	0	100	100
2	B	105/109 (96%)	100 (95%)	5 (5%)	0	100	100
2	D	100/109 (92%)	91 (91%)	9 (9%)	0	100	100
All	All	329/348 (94%)	313 (95%)	14 (4%)	2 (1%)	21	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	LEU
1	A	383	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	58/58 (100%)	56 (97%)	2 (3%)	32	35
1	C	56/58 (97%)	53 (95%)	3 (5%)	20	18
2	B	101/101 (100%)	99 (98%)	2 (2%)	48	56
2	D	97/101 (96%)	95 (98%)	2 (2%)	47	54
All	All	312/318 (98%)	303 (97%)	9 (3%)	37	42

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

Mol	Chain	Res	Type
1	A	357	ASP
1	A	372	LEU
2	B	16	GLN
2	B	50	LEU
1	C	347	ARG
1	C	353	THR
1	C	372	LEU
2	D	54	GLU
2	D	62	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	ASN
1	A	350	HIS
2	B	19	HIS
2	B	85	GLN
2	B	86	ASN
2	B	105	ASN
1	C	326	ASN
1	C	327	GLN
1	C	362	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
4	DDQ	A	102	-	11,13,13	1.17	1 (9%)	12,15,15	0.60	0
4	DDQ	C	105	-	11,13,13	1.10	1 (9%)	12,15,15	0.72	0
4	DDQ	A	104	-	11,13,13	1.16	2 (18%)	12,15,15	0.60	0
4	DDQ	C	108	-	11,13,13	1.19	2 (18%)	12,15,15	0.69	0
4	DDQ	A	101	-	11,13,13	1.15	1 (9%)	12,15,15	0.65	0
4	DDQ	B	120	-	11,13,13	1.17	2 (18%)	12,15,15	0.55	0
4	DDQ	B	119	-	11,13,13	1.16	2 (18%)	12,15,15	0.69	0
4	DDQ	D	119	-	11,13,13	1.24	1 (9%)	12,15,15	0.61	0

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	DDQ	A	102	-	-	4/11/11/11	-
4	DDQ	C	105	-	-	6/11/11/11	-
4	DDQ	A	104	-	-	5/11/11/11	-
4	DDQ	C	108	-	-	9/11/11/11	-
4	DDQ	A	101	-	-	4/11/11/11	-
4	DDQ	B	120	-	-	8/11/11/11	-
4	DDQ	B	119	-	-	2/11/11/11	-
4	DDQ	D	119	-	-	3/11/11/11	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	119	DDQ	C1-N1	-3.54	1.47	1.51
4	A	102	DDQ	C1-N1	-3.42	1.48	1.51
4	A	101	DDQ	C1-N1	-3.25	1.48	1.51
4	B	119	DDQ	C1-N1	-3.22	1.48	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	120	DDQ	C1-N1	-3.21	1.48	1.51
4	A	104	DDQ	C1-N1	-3.16	1.48	1.51
4	C	108	DDQ	C1-N1	-3.11	1.48	1.51
4	C	105	DDQ	C1-N1	-2.97	1.48	1.51
4	C	108	DDQ	O1-N1	2.17	1.47	1.42
4	A	104	DDQ	O1-N1	2.06	1.47	1.42
4	B	119	DDQ	O1-N1	2.02	1.47	1.42
4	B	120	DDQ	O1-N1	2.01	1.46	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	101	DDQ	C2-C1-N1-CM1
4	A	102	DDQ	N1-C1-C2-C3
4	A	104	DDQ	C2-C1-N1-CM1
4	A	104	DDQ	C2-C1-N1-CM2
4	B	120	DDQ	C2-C1-N1-CM2
4	C	108	DDQ	C2-C1-N1-CM2
4	C	108	DDQ	C5-C6-C7-C8
4	A	101	DDQ	C2-C3-C4-C5
4	D	119	DDQ	C5-C6-C7-C8
4	D	119	DDQ	C3-C4-C5-C6
4	C	105	DDQ	C5-C6-C7-C8
4	C	108	DDQ	C3-C4-C5-C6
4	D	119	DDQ	C4-C5-C6-C7
4	C	108	DDQ	C2-C3-C4-C5
4	A	102	DDQ	C4-C5-C6-C7
4	C	105	DDQ	C1-C2-C3-C4
4	C	105	DDQ	C2-C3-C4-C5
4	A	102	DDQ	C7-C8-C9-C10
4	A	104	DDQ	C7-C8-C9-C10
4	C	105	DDQ	C4-C5-C6-C7
4	A	104	DDQ	C3-C4-C5-C6
4	A	101	DDQ	C3-C4-C5-C6
4	B	120	DDQ	C3-C4-C5-C6
4	A	101	DDQ	C2-C1-N1-CM2
4	B	120	DDQ	C2-C1-N1-CM1
4	C	108	DDQ	C2-C1-N1-CM1
4	C	108	DDQ	C2-C1-N1-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	120	DDQ	C6-C7-C8-C9
4	C	108	DDQ	C4-C5-C6-C7
4	C	105	DDQ	C6-C7-C8-C9
4	B	120	DDQ	C2-C3-C4-C5
4	C	108	DDQ	C1-C2-C3-C4
4	B	119	DDQ	C7-C8-C9-C10
4	C	105	DDQ	C7-C8-C9-C10
4	C	108	DDQ	C7-C8-C9-C10
4	A	102	DDQ	C2-C1-N1-CM2
4	B	120	DDQ	C7-C8-C9-C10
4	B	120	DDQ	C1-C2-C3-C4
4	B	120	DDQ	C4-C5-C6-C7
4	B	119	DDQ	C3-C4-C5-C6
4	A	104	DDQ	C2-C1-N1-O1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	101	DDQ	3	0
4	B	119	DDQ	1	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, 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	65/65 (100%)	1.12	9 (13%) 6 6	53, 57, 64, 75	0
1	C	63/65 (96%)	1.07	7 (11%) 10 10	54, 57, 64, 68	0
2	B	107/109 (98%)	1.56	28 (26%) 1 1	53, 58, 61, 69	0
2	D	102/109 (93%)	1.84	34 (33%) 1 1	52, 58, 62, 63	0
All	All	337/348 (96%)	1.47	78 (23%) 2 2	52, 58, 63, 75	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	118	GLY	5.4
1	A	384	LEU	5.2
2	D	97	ILE	4.6
2	B	98	GLU	4.4
2	D	90	ILE	4.4
2	D	54	GLU	4.2
2	B	100	PHE	4.1
2	D	105	ASN	4.1
2	D	62	ILE	4.0
2	D	85	GLN	4.0
2	D	112	ILE	4.0
2	D	107	THR	3.9
2	D	113	THR	3.8
2	B	19	HIS	3.5
1	A	385	SER	3.5
1	C	383	PRO	3.4
2	D	94	PHE	3.4
2	D	111	ALA	3.3
2	D	35	GLU	3.3
2	D	61	SER	3.3
2	B	94	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	357	ASP	3.2
1	A	336	TYR	3.2
2	B	12	MET	3.2
2	D	83	ASN	3.2
1	C	323	ASP	3.1
2	D	59	LYS	3.1
2	D	92	LYS	3.1
2	D	60	ASP	3.1
2	B	102	ASP	3.1
2	B	85	GLN	3.1
2	D	89	GLU	3.1
2	D	96	SER	3.1
2	B	72	ASP	3.0
2	D	102	ASP	3.0
2	B	68	THR	2.8
2	D	80	VAL	2.8
2	B	38	GLU	2.8
2	B	41	SER	2.7
2	B	103	THR	2.7
2	D	106	ILE	2.7
1	A	378	GLN	2.7
2	B	25	PHE	2.7
2	B	115	LEU	2.6
2	B	57	TYR	2.6
2	B	97	ILE	2.6
1	A	340	ASP	2.6
2	D	27	ASN	2.5
1	A	325	LEU	2.5
2	B	13	ASP	2.4
2	D	72	ASP	2.4
1	C	354	ILE	2.4
2	D	84	SER	2.4
1	C	353	THR	2.4
1	A	322	THR	2.4
1	C	344	ALA	2.3
2	D	108	ALA	2.3
1	C	350	HIS	2.3
2	B	22	VAL	2.3
2	D	110	ASN	2.3
1	A	350	HIS	2.2
2	B	15	SER	2.2
2	B	21	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	31	SER	2.2
2	D	115	LEU	2.2
2	B	18	PHE	2.1
1	C	346	SER	2.1
2	D	101	ALA	2.1
2	D	58	LEU	2.1
2	B	81	TYR	2.1
2	D	100	PHE	2.1
2	B	99	ALA	2.1
2	D	28	SER	2.1
2	B	69	ASN	2.0
2	B	60	ASP	2.0
2	B	114	ARG	2.0
2	D	18	PHE	2.0
2	D	44	TYR	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 oligosaccharides 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
4	DDQ	C	108	14/14	0.57	0.22	100,103,106,106	0
4	DDQ	C	105	14/14	0.61	0.22	75,81,87,87	0
4	DDQ	B	120	14/14	0.65	0.21	74,75,79,79	0
4	DDQ	A	104	14/14	0.69	0.19	83,86,91,91	0
4	DDQ	B	119	14/14	0.72	0.18	64,71,80,80	0
4	DDQ	D	119	14/14	0.76	0.18	71,73,76,76	0
4	DDQ	A	101	14/14	0.78	0.17	70,73,79,79	0
4	DDQ	A	102	14/14	0.83	0.16	57,60,72,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	109	1/1	0.91	0.38	62,62,62,62	1

6.5 Other polymers [i](#)

There are no such residues in this entry.