



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:53 PM UTC

PDB ID : 7ASV / pdb_00007asv
Title : Crystal structure of tWHD2 of Rpc5 subunit of human RNA Polymerase III
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Deposited on : 2020-10-28
Resolution : 1.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

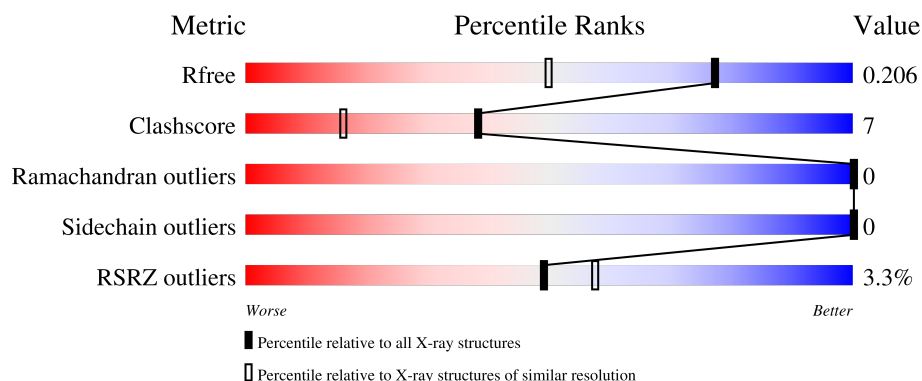
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	708	19% 78%
1	B	708	20% 78%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5622 atoms, of which 2569 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.

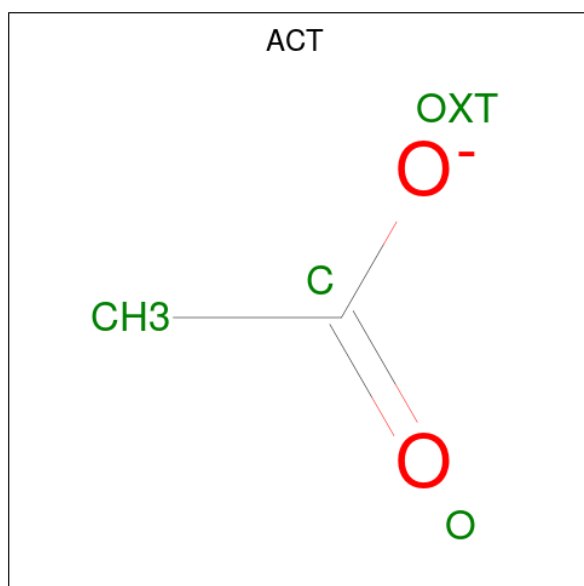
- Molecule 1 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	B	155	Total	C	H	N	O	S	Se	0	8	0
			2537	798	1276	221	233	5	4			
1	A	155	Total	C	H	N	O	S	Se	0	9	0
			2553	803	1287	222	231	5	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	555	PRO	SER	conflict	UNP Q9NVU0
A	555	PRO	SER	conflict	UNP Q9NVU0

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		

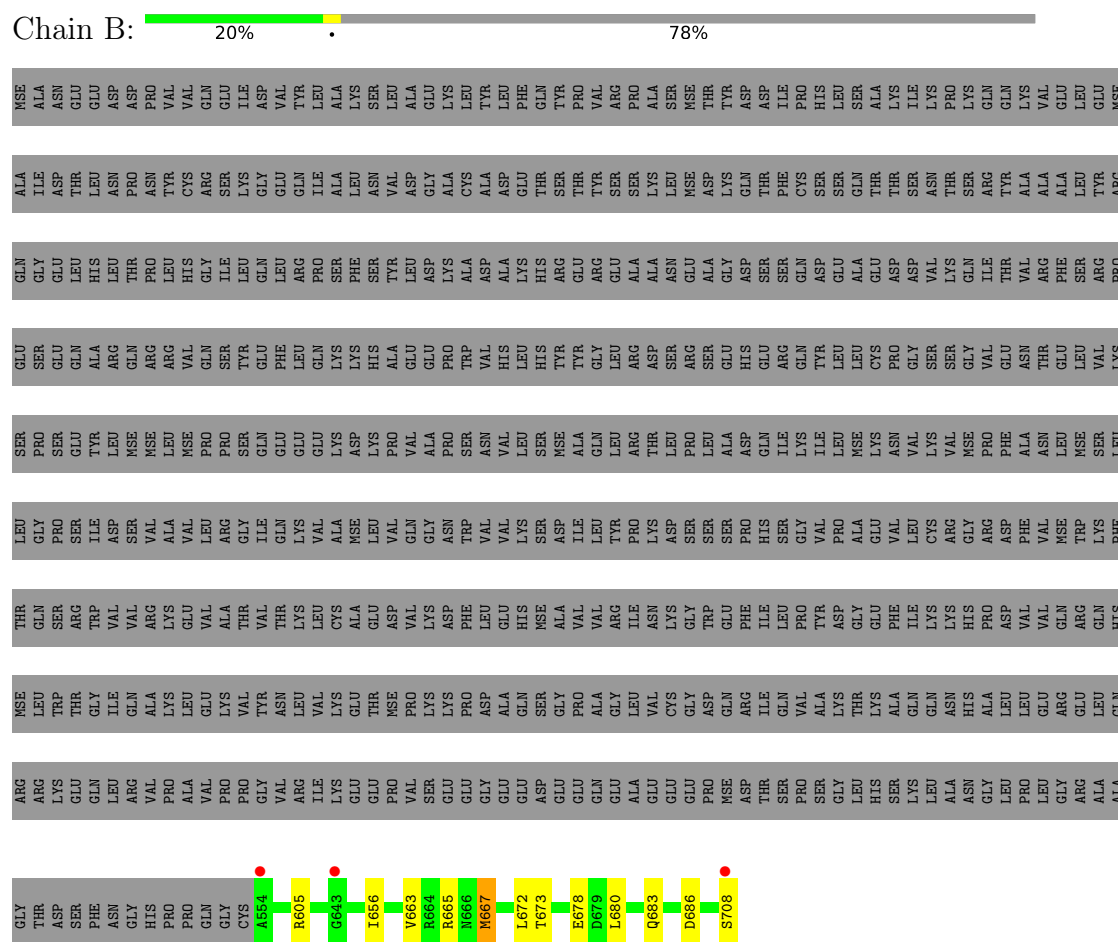
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	277	Total	O	0	0
			277	277		
3	A	241	Total	O	0	0
			241	241		

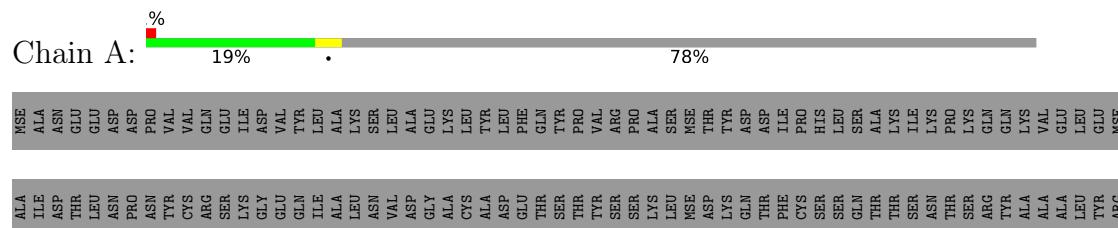
3 Residue-property plots

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: DNA-directed RNA polymerase III subunit RPC5



• Molecule 1: DNA-directed RNA polymerase III subunit RPC5



GLY	THR	ARG	MSE	THR	LEU	GLY	SER	GLN	GLY
THR	ARG	LYS	LEU	GLN	THR	GLY	PRO	GLY	GLY
ASP	LYS	GLU	THR	SER	THR	SER	GLU	GLU	SER
PHE	GLN	GLY	ILE	TRP	GLY	ILE	ALA	ALA	ALA
ASN	LEU	LEU	ILE	VAL	VAL	SER	ARG	THR	LEU
GLY	ARG	ARG	GLN	VAL	VAL	MSE	GLN	THR	THR
HIS	VAL	VAL	ALA	ARG	GLY	VAL	ARG	PRO	PRO
PRO	PRO	ALA	LYS	GLY	LEU	VAL	VAL	HIS	HIS
PRO	ALA	VAL	LEU	GLY	VAL	LEU	GLN	GLY	GLY
GLN	VAL	VAL	LYS	ALA	THR	ARG	SER	ILE	ILE
CYS	PRO	PRO	VAL	THR	GLY	GLY	TYR	TYR	LEU
A554	GLY	GLY	TYR	VAL	ILE	ILE	GLN	GLY	GLN
P555	VAL	VAL	ASN	THR	GLN	GLY	PHE	GLY	LEU
T556	ARG	ILE	LEU	LYS	LYS	LYS	LEU	ARG	ARG
	ILE	LYS	VAL	LEU	VAL	VAL	GLY	PRO	VAL
H596	LYS	GLY	LYS	CYS	ALA	ALA	LYS	LYS	PRO
T597	GLY	GLY	THR	ALA	GLY	MSE	ASP	ASP	PHE
	GLY	GLY	THR	GLY	GLY	LEU	LYS	TRP	ALA
S600	PRO	PRO	MSE	LEU	ASP	VAL	PRO	VAL	ASP
	VAL	VAL	PRO	VAL	GLY	VAL	ALA	HIS	ALA
D644	SER	GLY	LYS	GLY	ALA	GLY	GLY	LEU	ALA
M645	GLY	GLY	LYS	ASP	PRO	TRP	PRO	TRP	LYS
S646	GLY	GLY	ASP	LEU	ASP	VAL	SER	VAL	ASP
D647	GLY	GLY	ALA	GLY	ALA	VAL	ASN	VAL	ALA
Q648	GLY	GLY	GLN	GLY	GLY	VAL	VAL	HIS	ALA
H649	GLY	GLY	GLY	GLY	GLY	LYS	LEU	LYS	LYS
R650	GLY	GLY	SER	MSE	SER	GLY	HIS	HIS	HIS
	GLY	GLY	GLY	ALA	ASP	ASP	TYR	ARG	ARG
L653	GLY	GLY	PRO	VAL	PRO	ILE	ALA	GLY	GLY
	GLN	GLY	ALA	VAL	ALA	LEU	GLN	ARG	ARG
R662	GLY	GLY	GLY	ARG	GLY	TYR	LEU	GLY	GLY
	ALA	GLY	LEU	ILE	ILE	PRO	ARG	ALA	ALA
R665	GLY	GLY	VAL	ASN	VAL	LYS	THR	ASP	ALA
	GLY	GLY	CYS	LYS	CYS	ASP	LEU	ASN	ASN
Q669	GLY	GLY	ASP	TRP	SER	SER	PRO	ARG	GLY
	PRO	MSE	GLN	GLY	GLY	SER	LEU	SER	ALA
C676	ASP	ASP	ARG	PRO	SER	PRO	ALA	GLY	GLY
G677	THR	THR	ILE	ILE	ILE	GLY	HIS	ASP	ASP
E678	SER	SER	GLN	LEU	GLN	SER	GLY	SER	SER
D679	PRO	PRO	VAL	PRO	VAL	PRO	LYS	GLN	GLN
L680	SER	SER	ALA	ALA	ALA	TYR	ILE	TYR	ASP
S681	GLY	LEU	LYS	LYS	LYS	PRO	LEU	LEU	GLY
R682	LEU	HIS	THR	THR	GLY	ASP	MSE	LEU	ALA
Q683	HIS	LYS	LYS	GLY	GLY	GLY	LYS	CYS	GLY
E684	SER	LYS	ALA	PHE	VAL	VAL	ASN	PRO	ASP
V685	LEU	LYS	GLN	ILE	ILE	LEU	VAL	GLY	ASP
D686	LEU	GLY	GLN	LYS	LYS	CYS	VAL	ASP	VAL
R687	ALA	ASN	GLN	LYS	LYS	ARG	SER	SER	LYS
V688	GLY	HIS	ASN	HIS	GLY	GLY	VAL	SER	GLY
	GLY	LEU	ALA	PRO	ARG	ARG	ILE	VAL	GLN
D691	LEU	LEU	ALA	ASP	THR	THR	VAL	VAL	ILE
C692	PRO	LEU	LEU	VAL	VAL	PHE	ASP	GLY	THR
	LEU	GLY	LEU	VAL	VAL	VAL	ALA	ASN	THR
M699	GLY	LEU	ARG	GLN	GLN	MSE	LEU	THR	ARG
	ARG	ALA	GLY	LEU	TRP	TRP	LEU	GLY	PHE
S708	ALA	ALA	LEU	GLN	LYS	SER	VAL	VAL	ARG
									PRO

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.11Å 75.76Å 62.40Å 90.00° 103.57° 90.00°	Depositor
Resolution (Å)	30.33 – 1.55 30.33 – 1.55	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.33-1.55) 99.1 (30.33-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.48Å)	Xtriage
Refinement program	PHENIX phenix-1.18.1-3865	Depositor
R, R_{free}	0.180 , 0.210 0.174 , 0.206	Depositor DCC
R_{free} test set	2918 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5622	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.53% 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

5.1 Standard geometry

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

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	0.47	0/1318	0.61	0/1771
1	B	0.53	1/1309 (0.1%)	0.63	0/1758
All	All	0.51	1/2627 (0.0%)	0.62	0/3529

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	667	MSE	SE-CE	-5.29	1.79	1.95

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	676	CME	Mainchain

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	1266	1287	1242	24	0
1	B	1261	1276	1235	11	0
2	A	4	3	3	0	0
2	B	4	3	3	0	0
3	A	241	0	0	5	0
3	B	277	0	0	1	1
All	All	3053	2569	2483	35	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 7.

The worst 5 of 35 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:B:665[B]:ARG:NH2	1:B:686:ASP:OD2	2.09	0.84
1:A:688[B]:VAL:HG22	3:A:1038:HOH:O	1.82	0.79
1:A:556:THR:O	1:A:597:THR:HG21	1.84	0.77
1:B:656:ILE:HG21	1:B:667:MSE:HE1	1.74	0.69
1:B:656:ILE:CG2	1:B:667:MSE:HE1	2.23	0.68

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:B:1001:HOH:O	3:B:1125:HOH:O[2_657]	2.17	0.03

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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	161/708 (23%)	157 (98%)	4 (2%)	0	100	100
1	B	160/708 (23%)	157 (98%)	3 (2%)	0	100	100
All	All	321/1416 (23%)	314 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	144/600 (24%)	144 (100%)	0	100	100
1	B	144/600 (24%)	144 (100%)	0	100	100
All	All	288/1200 (24%)	288 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	669	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CME	B	676	1	8,9,10	0.61	0	6,9,11	0.52	0
1	CME	A	676	1	8,9,10	0.75	0	6,9,11	0.88	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
1	CME	B	676	1	-	0/5/8/10	-
1	CME	A	676	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	676	CME	CZ-CE-SD-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	676	CME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	ACT	B	801	-	3,3,3	0.91	0	3,3,3	0.72	0
2	ACT	A	801	-	3,3,3	0.97	0	3,3,3	0.94	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 [i](#)

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	150/708 (21%)	-0.10	7 (4%) 36 44	13, 24, 54, 85	4 (2%)
1	B	150/708 (21%)	-0.31	3 (2%) 65 73	9, 22, 39, 60	4 (2%)
All	All	300/1416 (21%)	-0.20	10 (3%) 49 57	9, 23, 50, 85	8 (2%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	LEU	5.6
1	A	554	ALA	3.3
1	A	708	SER	3.2
1	B	708	SER	3.1
1	B	643	GLY	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CME	A	676	10/11	0.93	0.10	42,50,57,59	0
1	CME	B	676	10/11	0.98	0.07	18,27,48,49	0

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($\text{\AA}^2$)	Q<0.9
2	ACT	B	801	4/4	0.98	0.04	20,22,27,27	0
2	ACT	A	801	4/4	0.99	0.03	18,20,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.