



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:50 AM UTC

PDB ID : 2HHP / pdb_00002hhp
Title : Structure of yeast poly(A) polymerase in a closed conformation.
Authors : Bohm, A.; Toth, J.
Deposited on : 2006-06-28
Resolution : 1.80 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

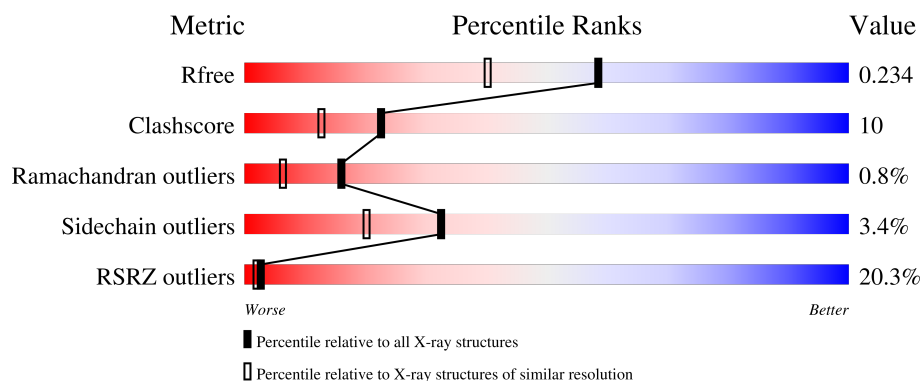
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	530	19% 77% 17% • •

2 Entry composition [i](#)

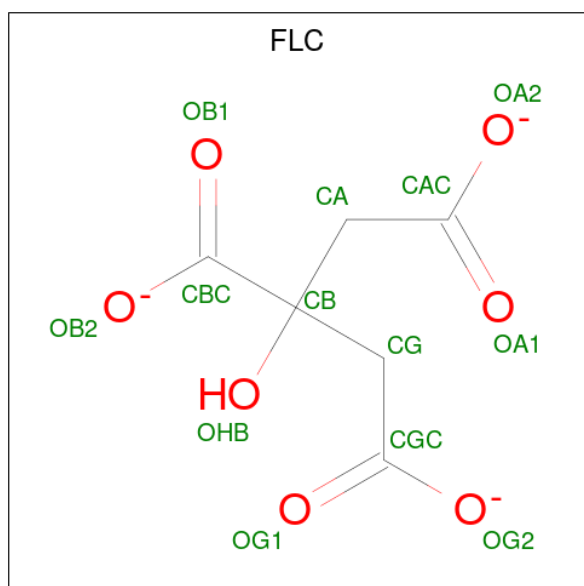
There are 4 unique types of molecules in this entry. The entry contains 4600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Poly(A) polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	27	0
			4193	2715	708	754	16			

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		

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

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

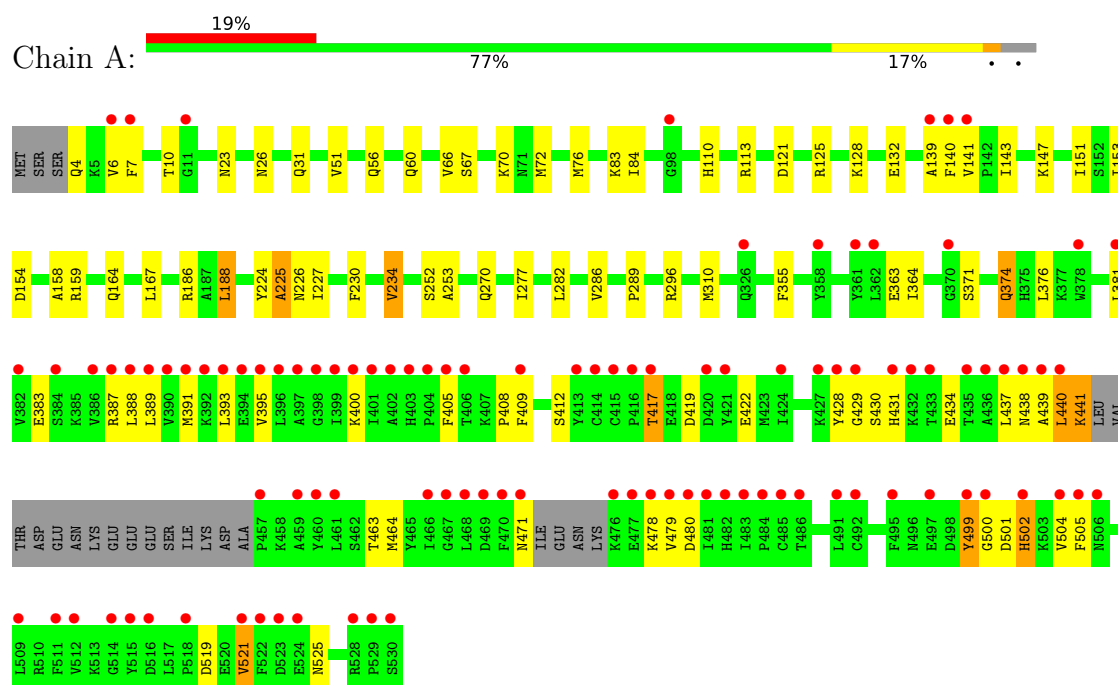
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	380	Total	O	0	0
			380	380		

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: Poly(A) polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.48Å 84.92Å 67.72Å 90.00° 111.78° 90.00°	Depositor
Resolution (Å)	33.04 – 1.80 33.04 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.04-1.80) 99.7 (33.04-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.99 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.197 , 0.236 0.196 , 0.234	Depositor DCC
R_{free} test set	2305 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.4	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	0.94	EDS
Total number of atoms	4600	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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: FLC, 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	0.90	1/4362 (0.0%)	0.98	1/5909 (0.0%)

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	A	422	GLU	C-N	5.26	1.41	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	TYR	N-CA-C	11.59	123.99	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	417	THR	Peptide

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	4193	0	4266	88	0
2	A	26	0	10	3	0
3	A	1	0	0	0	0
4	A	380	0	0	9	0
All	All	4600	0	4276	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387[B]:ARG:H	1:A:387[B]:ARG:HD3	1.07	1.15
1:A:387[B]:ARG:HH21	1:A:387[B]:ARG:HG3	1.11	1.09
1:A:478:LYS:HB3	1:A:479:VAL:HA	1.12	1.04
1:A:478:LYS:HB3	1:A:479:VAL:CA	1.90	1.01
1:A:387[B]:ARG:H	1:A:387[B]:ARG:CD	1.80	0.94
1:A:72:MET:HE3	1:A:76:MET:HE2	1.52	0.92
1:A:478:LYS:CB	1:A:479:VAL:HA	2.00	0.87
1:A:132:GLU:OE2	1:A:147[B]:LYS:NZ	2.07	0.86
1:A:389:LEU:O	1:A:393[A]:LEU:HD13	1.78	0.84
1:A:234[A]:VAL:HG23	2:A:532:FLC:OA1	1.79	0.82
1:A:417:THR:HB	1:A:419:ASP:H	1.46	0.80
1:A:227:ILE:O	1:A:387[B]:ARG:HD2	1.85	0.76
1:A:405:PHE:O	1:A:464[B]:MET:HE1	1.87	0.74
1:A:387[B]:ARG:HH21	1:A:387[B]:ARG:CG	1.96	0.70
1:A:501:ASP:O	1:A:502:HIS:HB2	1.91	0.70
1:A:387[B]:ARG:HG3	1:A:387[B]:ARG:NH2	1.90	0.69
1:A:67:SER:OG	1:A:110:HIS:HE1	1.75	0.69
1:A:26:ASN:HD22	1:A:253:ALA:H	1.43	0.67
1:A:147[B]:LYS:NZ	1:A:147[B]:LYS:HB2	2.09	0.66
1:A:289:PRO:O	1:A:296:ARG:HG3	1.96	0.66
1:A:23:ASN:HD22	2:A:531:FLC:CAC	2.15	0.59
1:A:140[A]:PHE:CZ	1:A:186[A]:ARG:HD3	2.37	0.59
1:A:387[B]:ARG:CG	1:A:387[B]:ARG:NH2	2.62	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:TYR:OH	1:A:463[A]:THR:HG21	2.02	0.59
1:A:227:ILE:O	1:A:387[B]:ARG:CD	2.52	0.57
1:A:499:TYR:N	1:A:500:GLY:HA3	2.18	0.57
1:A:417:THR:CB	1:A:419:ASP:H	2.17	0.56
1:A:56:GLN:HE22	1:A:84[A]:ILE:H	1.52	0.56
1:A:383:GLU:HG2	1:A:464[A]:MET:SD	2.46	0.56
1:A:4:GLN:HB2	1:A:7:PHE:CD1	2.41	0.56
1:A:66:VAL:O	1:A:70[A]:LYS:HG3	2.07	0.55
2:A:532:FLC:HA1	4:A:833:HOH:O	2.06	0.55
1:A:56:GLN:NE2	1:A:84[A]:ILE:H	2.05	0.55
1:A:10:THR:CG2	4:A:851:HOH:O	2.55	0.54
1:A:56:GLN:HE22	1:A:84[B]:ILE:H	1.55	0.54
1:A:121:ASP:OD2	1:A:125:ARG:HD2	2.08	0.54
1:A:56:GLN:HE22	1:A:83:LYS:HA	1.73	0.53
1:A:371:SER:O	1:A:374:GLN:NE2	2.41	0.53
1:A:56:GLN:NE2	1:A:84[B]:ILE:H	2.06	0.53
1:A:417:THR:HB	1:A:419:ASP:N	2.21	0.53
1:A:141:VAL:HG13	1:A:141:VAL:O	2.09	0.52
1:A:4:GLN:NE2	1:A:7:PHE:HE1	2.08	0.52
1:A:479:VAL:HG12	1:A:480:ASP:N	2.25	0.52
1:A:501:ASP:O	1:A:502:HIS:CB	2.58	0.51
1:A:4:GLN:HB2	1:A:7:PHE:CE1	2.48	0.48
1:A:128:LYS:HE3	4:A:840:HOH:O	2.13	0.48
1:A:437:LEU:O	1:A:438:ASN:HB2	2.14	0.48
1:A:158:ALA:CB	1:A:188:LEU:HD13	2.44	0.47
1:A:499:TYR:O	1:A:505:PHE:HB2	2.13	0.47
1:A:72:MET:HE3	1:A:76:MET:CE	2.35	0.47
1:A:140[A]:PHE:CE2	1:A:186[A]:ARG:HD3	2.50	0.46
1:A:113:ARG:NH1	4:A:785:HOH:O	2.48	0.46
1:A:431:HIS:HA	1:A:434:GLU:HG2	1.97	0.46
1:A:479:VAL:HG12	1:A:480:ASP:H	1.79	0.46
1:A:31[A]:GLN:HG2	4:A:796:HOH:O	2.15	0.46
1:A:10:THR:HG22	4:A:851:HOH:O	2.15	0.46
1:A:51:VAL:HG21	1:A:151[A]:ILE:HD12	1.98	0.45
1:A:409:PHE:HB2	1:A:463[A]:THR:CG2	2.47	0.45
1:A:400:LYS:HD2	1:A:471:ASN:HB3	1.99	0.45
1:A:355:PHE:CZ	1:A:521:VAL:HG22	2.52	0.44
1:A:388:LEU:HA	1:A:391:MET:HE3	1.98	0.44
1:A:440:LEU:HB3	1:A:441:LYS:CA	2.47	0.44
1:A:147[B]:LYS:HB2	1:A:147[B]:LYS:HZ2	1.83	0.44
1:A:439:ALA:HA	1:A:440:LEU:HA	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147[B]:LYS:HB2	1:A:147[B]:LYS:HZ3	1.80	0.43
1:A:143:ILE:HD11	1:A:154:ASP:HB3	2.01	0.43
1:A:277:ILE:CG2	1:A:286:VAL:HG11	2.50	0.42
1:A:60[B]:GLN:HG2	4:A:850:HOH:O	2.18	0.42
1:A:72:MET:HE2	1:A:76:MET:HB3	2.00	0.42
1:A:72:MET:CE	1:A:76:MET:HB3	2.50	0.42
1:A:110:HIS:CD2	1:A:110:HIS:H	2.37	0.42
1:A:381:LEU:HD22	1:A:499:TYR:CE2	2.54	0.42
1:A:310:MET:HG2	4:A:694:HOH:O	2.20	0.42
1:A:147[B]:LYS:NZ	1:A:147[B]:LYS:CB	2.81	0.42
1:A:226:ASN:HA	1:A:230:PHE:O	2.20	0.41
1:A:409:PHE:HB2	1:A:463[A]:THR:HG23	2.02	0.41
1:A:363:GLU:OE1	1:A:429:GLY:O	2.39	0.41
1:A:26:ASN:HD21	1:A:252:SER:HB2	1.85	0.41
1:A:430:SER:O	1:A:434:GLU:HB3	2.21	0.40
1:A:159[B]:ARG:NH1	4:A:774:HOH:O	2.53	0.40
1:A:51:VAL:CG2	1:A:151[A]:ILE:HD12	2.52	0.40
1:A:141:VAL:O	1:A:141:VAL:CG1	2.69	0.40
1:A:224:TYR:O	1:A:225:ALA:HB2	2.22	0.40
1:A:364:ILE:O	1:A:463[A]:THR:HA	2.21	0.40
1:A:408:PRO:HB3	1:A:464[A]:MET:SD	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	529/530 (100%)	509 (96%)	16 (3%)	4 (1%)	16 6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ALA
1	A	225	ALA
1	A	502	HIS
1	A	525	ASN

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	465/472 (98%)	449 (97%)	16 (3%)	32	20

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	164	GLN
1	A	167	LEU
1	A	188	LEU
1	A	234[A]	VAL
1	A	234[B]	VAL
1	A	270	GLN
1	A	282	LEU
1	A	374	GLN
1	A	376	LEU
1	A	412	SER
1	A	440	LEU
1	A	441	LYS
1	A	504	VAL
1	A	519	ASP
1	A	521	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	23	ASN

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Mol	Chain	Res	Type
1	A	26	ASN
1	A	43	GLN
1	A	56	GLN
1	A	110	HIS
1	A	314	HIS
1	A	336	ASN
1	A	341	ASN
1	A	490	ASN

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 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
2	FLC	A	531	-	12,12,12	0.98	0	17,17,17	1.21	1 (5%)
2	FLC	A	532	3	12,12,12	1.26	1 (8%)	17,17,17	1.65	6 (35%)

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
2	FLC	A	531	-	-	6/16/16/16	-
2	FLC	A	532	3	-	0/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	532	FLC	CB-CBC	-2.76	1.50	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	531	FLC	OB2-CBC-CB	3.16	119.21	113.14
2	A	532	FLC	OB2-CBC-CB	2.90	118.70	113.14
2	A	532	FLC	CG-CB-CA	2.58	115.92	109.31
2	A	532	FLC	CB-CA-CAC	-2.37	107.43	113.92
2	A	532	FLC	CA-CB-CBC	-2.27	105.01	110.03
2	A	532	FLC	OB1-CBC-CB	-2.16	117.90	122.09
2	A	532	FLC	OA1-CAC-CA	-2.04	117.17	122.95

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	531	FLC	CG-CB-CBC-OB1
2	A	531	FLC	CG-CB-CBC-OB2
2	A	531	FLC	OHB-CB-CBC-OB1
2	A	531	FLC	OHB-CB-CBC-OB2
2	A	531	FLC	CA-CB-CBC-OB1
2	A	531	FLC	CA-CB-CBC-OB2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	531	FLC	1	0
2	A	532	FLC	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, 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	508/530 (95%)	0.88	103 (20%) 3 2	12, 27, 48, 60	27 (5%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	ILE	5.1
1	A	140[A]	PHE	4.9
1	A	390	VAL	4.9
1	A	428	TYR	4.7
1	A	470	PHE	4.7
1	A	499	TYR	4.6
1	A	387[A]	ARG	4.6
1	A	386	VAL	4.3
1	A	500	GLY	4.3
1	A	401	ILE	4.3
1	A	393[A]	LEU	4.2
1	A	515	TYR	4.2
1	A	399	ILE	4.1
1	A	406	THR	4.1
1	A	479	VAL	4.0
1	A	459	ALA	4.0
1	A	414	CYS	3.8
1	A	7	PHE	3.7
1	A	431	HIS	3.6
1	A	404	PRO	3.6
1	A	402	ALA	3.6
1	A	522	PHE	3.6
1	A	388	LEU	3.5
1	A	440	LEU	3.5
1	A	478	LYS	3.5
1	A	466	ILE	3.4
1	A	395[A]	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	398	GLY	3.4
1	A	467	GLY	3.4
1	A	415	CYS	3.3
1	A	461	LEU	3.3
1	A	468	LEU	3.3
1	A	370	GLY	3.3
1	A	437	LEU	3.3
1	A	6	VAL	3.2
1	A	457	PRO	3.2
1	A	432	LYS	3.2
1	A	397	ALA	3.2
1	A	511	PHE	3.2
1	A	529	PRO	3.1
1	A	381	LEU	3.1
1	A	483	ILE	3.1
1	A	421	TYR	3.0
1	A	391	MET	3.0
1	A	361	TYR	3.0
1	A	512	VAL	3.0
1	A	141	VAL	3.0
1	A	530	SER	3.0
1	A	481	ILE	2.9
1	A	495	PHE	2.9
1	A	358	TYR	2.9
1	A	392	LYS	2.9
1	A	396	LEU	2.9
1	A	521	VAL	2.8
1	A	362	LEU	2.8
1	A	413	TYR	2.8
1	A	405	PHE	2.7
1	A	476	LYS	2.7
1	A	524	GLU	2.7
1	A	403	HIS	2.7
1	A	460	TYR	2.7
1	A	417	THR	2.7
1	A	502	HIS	2.7
1	A	469	ASP	2.6
1	A	509	LEU	2.6
1	A	139	ALA	2.6
1	A	416	PRO	2.5
1	A	436	ALA	2.5
1	A	504	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	518	PRO	2.5
1	A	505	PHE	2.5
1	A	382	VAL	2.5
1	A	435	THR	2.4
1	A	477	GLU	2.4
1	A	427	LYS	2.4
1	A	514	GLY	2.4
1	A	384	SER	2.4
1	A	480	ASP	2.3
1	A	523	ASP	2.3
1	A	420	ASP	2.3
1	A	485	CYS	2.3
1	A	497	GLU	2.3
1	A	394	GLU	2.3
1	A	492	CYS	2.3
1	A	491	LEU	2.3
1	A	389	LEU	2.3
1	A	400	LYS	2.2
1	A	486	THR	2.2
1	A	409	PHE	2.2
1	A	528	ARG	2.2
1	A	429	GLY	2.2
1	A	439	ALA	2.2
1	A	506	ASN	2.1
1	A	378	TRP	2.1
1	A	471	ASN	2.1
1	A	433	THR	2.1
1	A	438	ASN	2.1
1	A	516	ASP	2.1
1	A	482	HIS	2.1
1	A	11	GLY	2.0
1	A	326	GLN	2.0
1	A	98	GLY	2.0
1	A	484	PRO	2.0

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

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($\text{\AA}^2$)	Q<0.9
2	FLC	A	531	13/13	0.57	0.20	82,84,84,85	0
2	FLC	A	532	13/13	0.71	0.17	70,72,74,75	0
3	MG	A	533	1/1	0.88	0.12	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.