



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:49 PM EST

PDB ID : 5LQE
Title : CDK2/Cyclin A in complex with compound 73
Authors : Coxon, C.R.; Anscombe, E.; Harnor, S.J.; Martin, M.P.; Carbain, B.; Hardcastle, I.R.; Harlow, L.K.; Korolchuk, S.; Matheson, C.J.; Noble, M.E.M.; Newell, D.R.; Turner, D.; Sivaprakasam, M.; Wang, L.Z.; Wong, C.; Golding, B.T.; Griffin, R.J.; Cano, G.
Deposited on : 2016-08-17
Resolution : 2.97 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-20028442
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-20028442

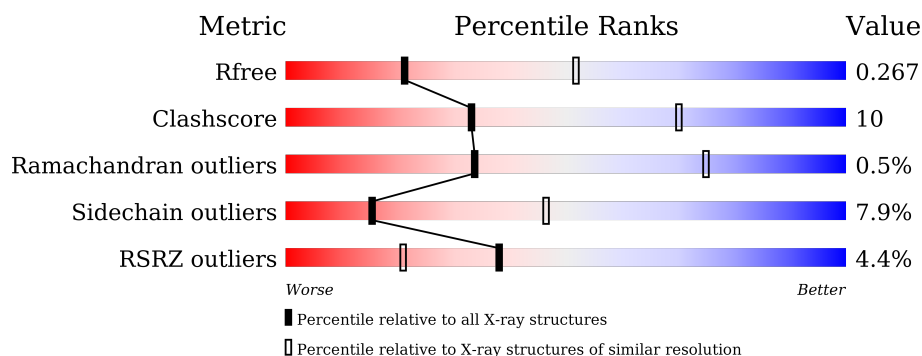
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	303	<div> <div>2%</div> <div>79%</div> <div>14%</div> <div>• •</div> </div>
1	C	303	<div> <div>4%</div> <div>74%</div> <div>21%</div> <div>• • •</div> </div>
2	B	260	<div> <div>2%</div> <div>80%</div> <div>17%</div> <div>• •</div> </div>
2	D	260	<div> <div>10%</div> <div>72%</div> <div>23%</div> <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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	72L	A	301	-	X	X	X
3	72L	C	301	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8992 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	P	S	0	0	0
			2380	1544	403	424	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2381	1544	404	424	1	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P24941
A	-3	PRO	-	expression tag	UNP P24941
A	-2	LEU	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-4	GLY	-	expression tag	UNP P24941
C	-3	PRO	-	expression tag	UNP P24941
C	-2	LEU	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

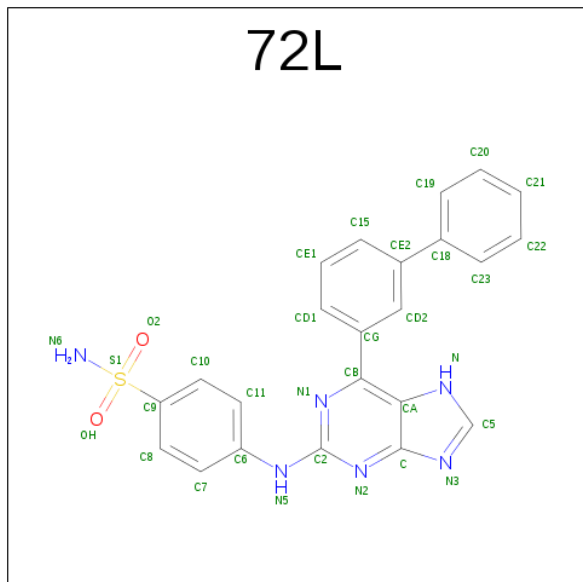
- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	0	0
			2075	1344	338	382	11			
2	D	257	Total	C	N	O	S	0	0	0
			2075	1344	338	382	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	MET	-	initiating methionine	UNP P20248
D	173	MET	-	initiating methionine	UNP P20248

- Molecule 3 is 4-[[6-(3-phenylphenyl)-7 {H}-purin-2-yl]amino]benzenesulfonamide (three-letter code: 72L) (formula: C₂₃H₁₈N₆O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	23	6	2	1		
3	C	1	Total	C	N	O	S	0	0
			32	23	6	2	1		

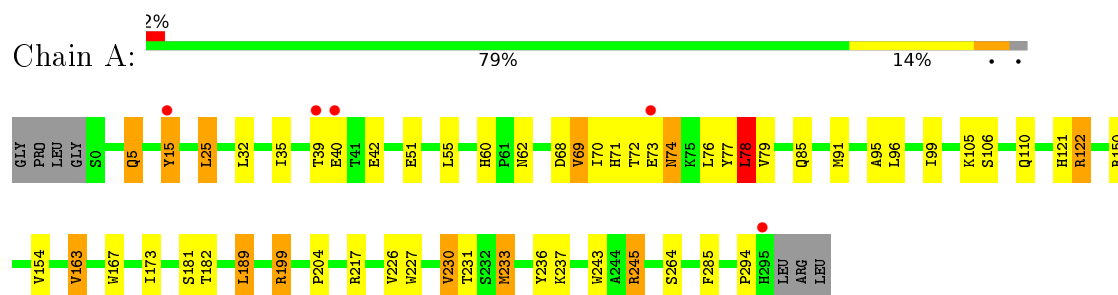
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	2	Total	O	0	0
			2	2		
4	C	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		

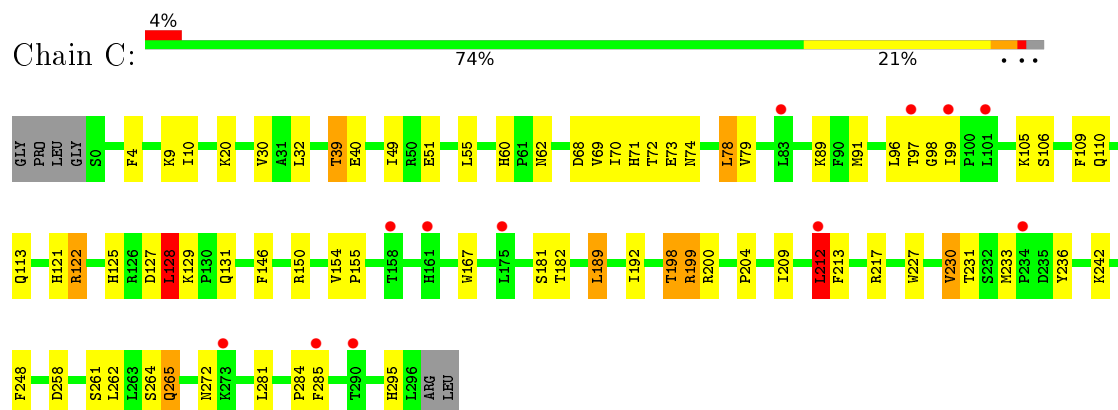
3 Residue-property plots [i](#)

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.

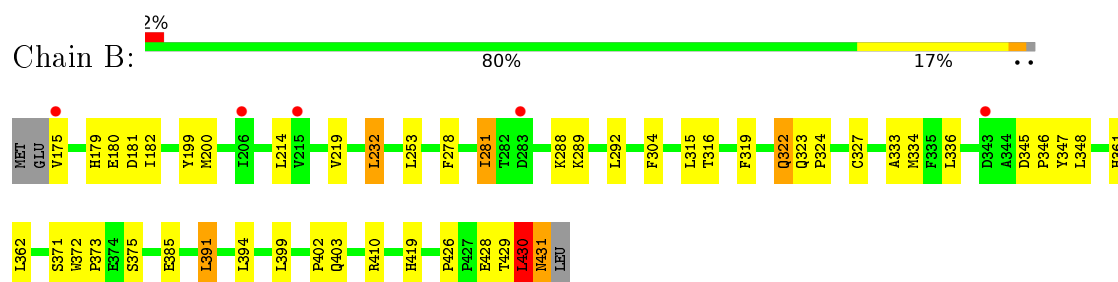
• Molecule 1: Cyclin-dependent kinase 2



• Molecule 1: Cyclin-dependent kinase 2

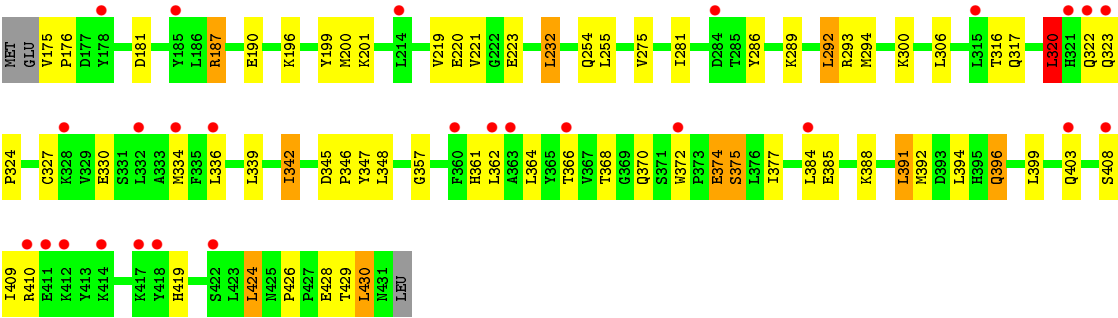


• Molecule 2: Cyclin-A2



• Molecule 2: Cyclin-A2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.53Å 132.05Å 149.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.03 – 2.97 66.03 – 2.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.03-2.97) 100.0 (66.03-2.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.213 , 0.266 0.213 , 0.267	Depositor DCC
R_{free} test set	1544 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8992	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 3.43% 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: TPO, 72L

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	0.60	0/2430	0.83	3/3297 (0.1%)
1	C	0.58	1/2430 (0.0%)	0.83	4/3297 (0.1%)
2	B	0.55	0/2125	0.80	1/2886 (0.0%)
2	D	0.55	0/2125	0.78	2/2886 (0.1%)
All	All	0.57	1/9110 (0.0%)	0.81	10/12366 (0.1%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	265	GLN	CD-NE2	5.07	1.45	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	212	LEU	CA-CB-CG	7.97	133.64	115.30
1	C	78	LEU	CA-CB-CG	7.34	132.19	115.30
1	A	78	LEU	CA-CB-CG	6.81	130.97	115.30
2	D	320	LEU	CA-CB-CG	6.28	129.75	115.30
1	A	69	VAL	CG1-CB-CG2	-6.25	100.91	110.90
1	C	128	LEU	CA-CB-CG	6.03	129.18	115.30
2	D	187	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	212	LEU	CB-CG-CD1	5.58	120.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	430	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	25	LEU	CB-CG-CD2	5.39	120.17	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	295	HIS	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	2380	0	2419	70	0
1	C	2381	0	2423	52	1
2	B	2075	0	2096	27	0
2	D	2075	0	2096	43	1
3	A	32	0	0	44	0
3	C	32	0	0	17	0
4	A	12	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
All	All	8992	0	9034	186	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 10.

All (186) 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:69:VAL:HG12	3:A:301:72L:C15	1.59	1.32
1:A:68:ASP:O	3:A:301:72L:OH	1.52	1.25
1:A:69:VAL:O	3:A:301:72L:CG	1.86	1.23
1:A:69:VAL:C	3:A:301:72L:CD2	2.09	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HG	3:A:301:72L:C23	1.69	1.21
2:B:175:VAL:O	2:B:179:HIS:HB2	1.37	1.20
1:A:69:VAL:O	3:A:301:72L:N1	1.92	1.03
1:A:78:LEU:HD23	3:A:301:72L:C20	1.88	1.03
1:A:69:VAL:O	3:A:301:72L:CD2	2.05	1.02
1:A:69:VAL:O	3:A:301:72L:CB	2.07	1.01
1:A:68:ASP:HB3	3:A:301:72L:C9	1.92	0.97
1:A:70:ILE:N	3:A:301:72L:CD2	2.29	0.95
1:A:69:VAL:HG12	3:A:301:72L:CE1	2.03	0.89
1:A:70:ILE:C	3:A:301:72L:CD2	2.41	0.89
1:A:79:VAL:N	3:A:301:72L:N6	2.21	0.88
1:A:69:VAL:HG12	3:A:301:72L:CE2	2.03	0.88
1:A:69:VAL:CG1	3:A:301:72L:C15	2.52	0.88
1:A:76:LEU:CG	3:A:301:72L:C23	2.53	0.85
1:A:70:ILE:HG13	3:A:301:72L:C7	2.07	0.85
1:C:125:HIS:ND1	1:C:128:LEU:HD23	1.95	0.81
3:A:301:72L:CE1	2:B:304:PHE:CE2	2.65	0.80
1:A:70:ILE:CA	3:A:301:72L:CD2	2.59	0.79
1:A:79:VAL:N	3:A:301:72L:S1	2.53	0.79
1:C:105:LYS:HE2	1:C:285:PHE:O	1.84	0.78
1:A:70:ILE:HA	3:A:301:72L:N1	1.99	0.78
2:D:364:LEU:CD2	2:D:370:GLN:HB2	2.13	0.78
1:C:60:HIS:HD2	1:C:62:ASN:H	1.31	0.77
1:A:60:HIS:HD2	1:A:62:ASN:H	1.31	0.76
1:A:105:LYS:HE2	1:A:285:PHE:O	1.85	0.76
1:A:78:LEU:CD2	3:A:301:72L:C20	2.64	0.74
1:A:70:ILE:HG13	3:A:301:72L:C6	2.17	0.74
1:C:69:VAL:HB	3:C:301:72L:O2	1.88	0.73
2:B:175:VAL:O	2:B:179:HIS:CB	2.30	0.73
1:A:68:ASP:HB3	3:A:301:72L:C10	2.18	0.72
1:A:69:VAL:CG1	3:A:301:72L:CE1	2.68	0.72
1:A:69:VAL:N	3:A:301:72L:C8	2.53	0.70
1:C:209:ILE:HD12	1:C:212:LEU:HD21	1.75	0.69
1:C:69:VAL:O	3:C:301:72L:O2	2.10	0.69
2:D:199:TYR:CE2	2:D:348:LEU:HD21	2.27	0.69
2:D:199:TYR:HE2	2:D:348:LEU:HD21	1.58	0.67
3:C:301:72L:C7	3:C:301:72L:N1	2.55	0.67
1:A:68:ASP:HB3	3:A:301:72L:C8	2.25	0.66
1:A:245:ARG:HH11	1:A:245:ARG:HG3	1.60	0.66
1:C:261:SER:OG	1:C:265:GLN:NE2	2.28	0.66
1:A:154:VAL:O	2:B:316:THR:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASP:C	3:A:301:72L:OH	2.33	0.65
1:A:95:ALA:O	1:A:199:ARG:NH1	2.26	0.65
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.32	0.65
1:A:78:LEU:HD23	3:A:301:72L:C19	2.28	0.64
1:C:70:ILE:HG23	3:C:301:72L:C21	2.28	0.64
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.33	0.63
1:C:213:PHE:O	1:C:217:ARG:HG3	1.99	0.62
1:C:227:TRP:O	1:C:230:VAL:HG22	1.99	0.62
2:D:339:LEU:O	2:D:342:ILE:HG12	2.00	0.62
2:D:339:LEU:HA	2:D:342:ILE:HD11	1.81	0.62
1:C:71:HIS:O	3:C:301:72L:C22	2.47	0.62
1:C:91:MET:HG2	1:C:99:ILE:HD11	1.82	0.62
2:D:364:LEU:HD22	2:D:370:GLN:HB2	1.80	0.62
2:D:396:GLN:HA	2:D:396:GLN:NE2	2.15	0.61
1:A:227:TRP:O	1:A:230:VAL:HG22	2.00	0.61
1:A:40:GLU:OE2	2:B:288:LYS:HE2	2.00	0.61
1:C:69:VAL:O	3:C:301:72L:S1	2.59	0.60
2:B:402:PRO:HA	2:B:410:ARG:HH21	1.66	0.60
1:A:79:VAL:N	3:A:301:72L:OH	2.31	0.60
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.84	0.59
1:C:69:VAL:O	3:C:301:72L:N6	2.37	0.58
1:A:51:GLU:O	1:A:55:LEU:HB2	2.03	0.58
1:C:60:HIS:CD2	1:C:62:ASN:H	2.18	0.58
1:A:79:VAL:HG23	3:A:301:72L:N6	2.20	0.57
1:C:98:GLY:N	1:C:199:ARG:HH21	2.02	0.57
1:C:51:GLU:O	1:C:55:LEU:HB2	2.05	0.56
2:D:364:LEU:HD21	2:D:370:GLN:HB2	1.86	0.56
1:C:198:THR:O	1:C:200:ARG:N	2.39	0.56
1:A:60:HIS:CD2	1:A:62:ASN:H	2.18	0.56
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.87	0.56
1:A:78:LEU:CD2	3:A:301:72L:C19	2.84	0.55
1:A:71:HIS:N	3:A:301:72L:CD2	2.70	0.55
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.89	0.55
2:D:409:ILE:HD12	2:D:409:ILE:H	1.72	0.55
3:A:301:72L:CE1	2:B:304:PHE:CZ	2.89	0.55
2:D:175:VAL:N	2:D:176:PRO:HD3	2.22	0.55
1:C:113:GLN:HG2	1:C:281:LEU:HD21	1.89	0.54
2:D:254:GLN:HG2	2:D:286:TYR:HE2	1.73	0.53
1:A:25:LEU:HD11	2:D:293:ARG:HB3	1.90	0.53
2:B:399:LEU:HD23	2:B:426:PRO:HB2	1.91	0.52
2:B:431:ASN:HD22	2:B:431:ASN:N	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:TYR:CE2	2:B:348:LEU:HD21	2.45	0.52
1:C:97:THR:C	1:C:199:ARG:HH21	2.13	0.52
1:C:10:ILE:HD11	1:C:20:LYS:HB2	1.92	0.51
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.26	0.51
1:C:32:LEU:HD23	1:C:79:VAL:HG22	1.92	0.51
1:A:68:ASP:C	3:A:301:72L:C8	2.79	0.51
1:C:189:LEU:HA	1:C:192:ILE:HD12	1.93	0.50
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.26	0.50
2:D:196:LYS:HG3	2:D:199:TYR:HB3	1.92	0.50
1:C:68:ASP:OD1	3:C:301:72L:OH	2.30	0.49
1:C:70:ILE:HA	3:C:301:72L:N6	2.26	0.49
1:C:155:PRO:HD3	2:D:320:LEU:HD12	1.94	0.49
1:C:106:SER:O	1:C:110:GLN:HG3	2.12	0.49
2:B:361:HIS:HD2	2:B:391:LEU:HD21	1.75	0.49
1:C:39:THR:O	2:D:292:LEU:HD23	2.13	0.49
1:A:106:SER:O	1:A:110:GLN:HG3	2.13	0.48
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.96	0.48
2:D:221:VAL:HG21	2:D:281:ILE:HD13	1.96	0.48
1:A:227:TRP:O	1:A:230:VAL:CG2	2.62	0.48
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.96	0.48
2:B:319:PHE:O	2:B:322:GLN:HB2	2.14	0.48
2:D:323:GLN:HA	2:D:324:PRO:HA	1.69	0.48
2:D:327:CYS:HB3	2:D:419:HIS:CE1	2.49	0.47
3:A:301:72L:N2	3:C:301:72L:CG	2.78	0.47
2:B:336:LEU:HD13	2:B:362:LEU:HD23	1.96	0.47
2:B:199:TYR:HE2	2:B:348:LEU:HD21	1.79	0.47
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.50	0.47
2:B:323:GLN:HA	2:B:324:PRO:HA	1.69	0.47
1:A:122:ARG:HB3	2:B:182:ILE:HG12	1.96	0.47
2:D:361:HIS:HD2	2:D:391:LEU:HD21	1.76	0.47
1:A:105:LYS:HE3	1:A:285:PHE:CE1	2.50	0.47
1:C:109:PHE:O	1:C:113:GLN:HG3	2.14	0.47
3:C:301:72L:CD1	2:D:300:LYS:HE2	2.44	0.47
1:C:32:LEU:CD2	1:C:79:VAL:HG22	2.45	0.46
2:D:275:VAL:HG21	2:D:292:LEU:HD11	1.97	0.46
2:B:327:CYS:HB3	2:B:419:HIS:CE1	2.51	0.46
1:C:227:TRP:O	1:C:230:VAL:CG2	2.62	0.46
1:C:167:TRP:CD1	1:C:204:PRO:HA	2.51	0.46
1:C:69:VAL:CA	3:C:301:72L:O2	2.63	0.46
2:D:317:GLN:O	2:D:320:LEU:CD2	2.63	0.46
2:D:317:GLN:O	2:D:320:LEU:HD22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LYS:HE3	1:C:285:PHE:CE1	2.51	0.45
1:A:71:HIS:N	3:A:301:72L:CG	2.79	0.45
1:A:73:GLU:HG2	1:A:74:ASN:HD22	1.81	0.45
2:D:399:LEU:HD23	2:D:426:PRO:HB2	1.98	0.45
1:C:69:VAL:CB	3:C:301:72L:O2	2.61	0.44
2:D:388:LYS:O	2:D:392:MET:HG2	2.17	0.44
1:A:181:SER:OG	1:A:182:THR:N	2.50	0.44
2:B:278:PHE:HA	2:B:281:ILE:CD1	2.47	0.44
2:D:187:ARG:HD2	2:D:187:ARG:HA	1.80	0.44
2:D:396:GLN:HE21	2:D:396:GLN:HA	1.82	0.44
2:B:372:TRP:HA	2:B:373:PRO:HD3	1.91	0.44
2:D:345:ASP:HA	2:D:346:PRO:HA	1.84	0.43
2:B:428:GLU:CD	2:B:428:GLU:H	2.22	0.43
1:C:49:ILE:HG23	2:D:306:LEU:HD12	2.00	0.43
1:C:69:VAL:C	3:C:301:72L:O2	2.56	0.43
2:B:347:TYR:OH	2:B:394:LEU:HA	2.18	0.43
1:C:4:PHE:CE1	1:C:30:VAL:HG21	2.54	0.43
1:C:181:SER:OG	1:C:182:THR:N	2.48	0.43
1:A:95:ALA:HA	1:A:199:ARG:CD	2.49	0.42
1:C:189:LEU:HA	1:C:189:LEU:HD23	1.89	0.42
2:D:357:GLY:HA2	2:D:372:TRP:CZ3	2.54	0.42
1:C:129:LYS:HE3	1:C:131:GLN:HB3	2.02	0.42
1:C:154:VAL:O	2:D:316:THR:HG22	2.19	0.42
1:A:189:LEU:HA	1:A:189:LEU:HD23	1.89	0.42
1:A:25:LEU:HD11	2:D:293:ARG:CB	2.48	0.42
1:A:71:HIS:H	3:A:301:72L:CB	2.32	0.42
2:B:278:PHE:HA	2:B:281:ILE:HD11	2.01	0.42
2:D:322:GLN:HE22	2:D:330:GLU:CG	2.32	0.42
2:D:347:TYR:OH	2:D:394:LEU:HA	2.19	0.42
1:C:231:THR:HA	1:C:236:TYR:CD2	2.55	0.42
1:A:230:VAL:O	1:A:233:MET:HB2	2.19	0.42
2:D:366:THR:HG22	2:D:424:LEU:HD22	2.02	0.42
1:A:121:HIS:O	1:A:122:ARG:HG3	2.20	0.41
1:A:231:THR:HA	1:A:236:TYR:CD2	2.55	0.41
1:A:15:TYR:HE1	1:A:35:ILE:HD11	1.85	0.41
1:C:258:ASP:OD2	1:C:284:PRO:HB2	2.20	0.41
1:A:69:VAL:N	3:A:301:72L:C7	2.83	0.41
3:A:301:72L:CB	3:C:301:72L:C5	2.93	0.41
2:D:223:GLU:OE1	2:D:223:GLU:HA	2.20	0.41
1:A:163:VAL:HG12	1:A:173:ILE:HD13	2.02	0.41
1:C:209:ILE:O	1:C:212:LEU:HD22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLN:HG3	1:A:5:GLN:O	2.20	0.41
1:C:127:ASP:O	1:C:128:LEU:C	2.59	0.41
2:D:220:GLU:HG3	2:D:408:SER:HB3	2.02	0.41
2:D:374:GLU:HG2	2:D:375:SER:N	2.36	0.41
2:D:255:LEU:HG	2:D:294:MET:HG2	2.03	0.41
1:A:32:LEU:HD22	1:A:77:TYR:CD1	2.56	0.41
1:C:51:GLU:HG3	1:C:146:PHE:HB2	2.02	0.41
1:C:69:VAL:N	3:C:301:72L:O2	2.54	0.40
1:A:217:ARG:HG2	1:A:243:TRP:CE2	2.56	0.40
1:A:69:VAL:HA	3:A:301:72L:C19	2.51	0.40
1:A:69:VAL:O	3:A:301:72L:CD1	2.62	0.40
2:B:315:LEU:HD22	2:B:333:ALA:HB1	2.03	0.40
1:C:262:LEU:HA	1:C:265:GLN:OE1	2.21	0.40
1:A:70:ILE:HA	3:A:301:72L:CB	2.51	0.40
2:B:345:ASP:HA	2:B:346:PRO:HA	1.83	0.40
1:C:121:HIS:O	1:C:122:ARG:HG3	2.21	0.40
1:C:69:VAL:C	3:C:301:72L:S1	3.00	0.40
2:D:364:LEU:HD23	2:D:368:THR:OG1	2.21	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)
1:C:9:LYS:O	2:D:403:GLN:NE2[3_455]	2.14	0.06

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	293/303 (97%)	281 (96%)	10 (3%)	2 (1%)	26 68
1	C	294/303 (97%)	282 (96%)	11 (4%)	1 (0%)	46 82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	255/260 (98%)	249 (98%)	5 (2%)	1 (0%)	39	79
2	D	255/260 (98%)	250 (98%)	4 (2%)	1 (0%)	39	79
All	All	1097/1126 (97%)	1062 (97%)	30 (3%)	5 (0%)	34	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ARG
1	C	199	ARG
1	A	294	PRO
2	B	430	LEU
2	D	430	LEU

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	260/265 (98%)	241 (93%)	19 (7%)	17	51
1	C	260/265 (98%)	240 (92%)	20 (8%)	16	48
2	B	231/234 (99%)	214 (93%)	17 (7%)	17	50
2	D	231/234 (99%)	209 (90%)	22 (10%)	11	36
All	All	982/998 (98%)	904 (92%)	78 (8%)	15	46

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	15	TYR
1	A	39	THR
1	A	42	GLU
1	A	72	THR
1	A	74	ASN
1	A	78	LEU

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Mol	Chain	Res	Type
1	A	85	GLN
1	A	96	LEU
1	A	122	ARG
1	A	150	ARG
1	A	163	VAL
1	A	189	LEU
1	A	226	VAL
1	A	230	VAL
1	A	233	MET
1	A	237	LYS
1	A	245	ARG
1	A	264	SER
2	B	180	GLU
2	B	181	ASP
2	B	200	MET
2	B	232	LEU
2	B	281	ILE
2	B	289	LYS
2	B	292	LEU
2	B	322	GLN
2	B	334	MET
2	B	371	SER
2	B	375	SER
2	B	385	GLU
2	B	391	LEU
2	B	403	GLN
2	B	429	THR
2	B	430	LEU
2	B	431	ASN
1	C	39	THR
1	C	40	GLU
1	C	72	THR
1	C	73	GLU
1	C	74	ASN
1	C	78	LEU
1	C	89	LYS
1	C	96	LEU
1	C	122	ARG
1	C	128	LEU
1	C	150	ARG
1	C	189	LEU
1	C	198	THR

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Mol	Chain	Res	Type
1	C	212	LEU
1	C	230	VAL
1	C	233	MET
1	C	242	LYS
1	C	248	PHE
1	C	264	SER
1	C	272	ASN
2	D	181	ASP
2	D	190	GLU
2	D	200	MET
2	D	201	LYS
2	D	232	LEU
2	D	289	LYS
2	D	292	LEU
2	D	320	LEU
2	D	334	MET
2	D	342	ILE
2	D	374	GLU
2	D	375	SER
2	D	377	ILE
2	D	384	LEU
2	D	385	GLU
2	D	391	LEU
2	D	396	GLN
2	D	410	ARG
2	D	424	LEU
2	D	428	GLU
2	D	429	THR
2	D	430	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	74	ASN
2	B	419	HIS
2	B	431	ASN
1	C	60	HIS
1	C	265	GLN
1	C	272	ASN
2	D	322	GLN

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Mol	Chain	Res	Type
2	D	323	GLN
2	D	396	GLN
2	D	419	HIS

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	TPO	A	160	1	7,10,11	0.62	0	10,14,16	1.18	0
1	TPO	C	160	1	7,10,11	0.64	0	10,14,16	1.05	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	TPO	A	160	1	-	0/8/11/13	0/0/0/0
1	TPO	C	160	1	-	0/8/11/13	0/0/0/0

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.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
3	72L	A	301	1,3	33,36,36	4.86	20 (60%)	43,52,52	7.23	34 (79%)
3	72L	C	301	3	33,36,36	3.26	14 (42%)	43,52,52	4.59	27 (62%)

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
3	72L	A	301	1,3	-	0/18/18/18	0/5/5/5
3	72L	C	301	3	-	0/18/18/18	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	72L	C9-S1	-5.90	1.68	1.77
3	A	301	72L	CE1-C15	-5.36	1.28	1.38
3	C	301	72L	C7-C8	-4.27	1.30	1.38
3	A	301	72L	C8-C9	-3.05	1.33	1.38
3	C	301	72L	C6-N5	-2.56	1.35	1.40
3	A	301	72L	C15-CE2	-2.52	1.34	1.39
3	C	301	72L	C11-C10	-2.44	1.34	1.38
3	A	301	72L	C7-C6	-2.36	1.35	1.39
3	C	301	72L	C8-C9	-2.33	1.35	1.38
3	C	301	72L	C21-C22	2.15	1.43	1.38
3	A	301	72L	C-N3	2.28	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	72L	CD2-CG	2.32	1.44	1.39
3	C	301	72L	CA-N	2.73	1.49	1.39
3	A	301	72L	C6-N5	2.92	1.46	1.40
3	C	301	72L	C20-C19	3.08	1.44	1.38
3	A	301	72L	CG-CB	3.25	1.53	1.49
3	A	301	72L	C10-C9	3.31	1.44	1.38
3	C	301	72L	C7-C6	3.43	1.44	1.39
3	A	301	72L	CA-N	3.48	1.51	1.39
3	A	301	72L	C11-C10	3.67	1.46	1.38
3	C	301	72L	CB-N1	4.22	1.36	1.32
3	A	301	72L	CE1-CD1	5.44	1.49	1.38
3	C	301	72L	OH-S1	5.46	1.50	1.43
3	A	301	72L	C11-C6	5.90	1.48	1.39
3	C	301	72L	C22-C23	6.15	1.50	1.38
3	A	301	72L	OH-S1	6.91	1.52	1.43
3	C	301	72L	S1-N6	7.59	1.73	1.60
3	A	301	72L	C20-C19	7.74	1.54	1.38
3	A	301	72L	C21-C20	7.81	1.57	1.38
3	A	301	72L	S1-N6	8.63	1.75	1.60
3	C	301	72L	C2-N5	9.04	1.53	1.36
3	A	301	72L	C22-C23	10.21	1.58	1.38
3	A	301	72L	C2-N5	10.57	1.56	1.36
3	A	301	72L	CB-N1	11.38	1.43	1.32

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	72L	O2-S1-OH	-25.11	85.13	118.87
3	A	301	72L	C22-C21-C20	-12.75	98.16	119.88
3	C	301	72L	O2-S1-C9	-12.55	93.27	107.41
3	A	301	72L	C8-C9-S1	-11.20	103.26	119.75
3	A	301	72L	N2-C2-N1	-10.30	110.77	126.18
3	A	301	72L	CD1-CG-CD2	-9.95	105.56	118.17
3	C	301	72L	C7-C8-C9	-8.47	110.46	119.49
3	C	301	72L	C8-C9-S1	-7.99	107.99	119.75
3	C	301	72L	C6-N5-C2	-7.00	111.69	129.34
3	C	301	72L	C22-C23-C18	-6.30	112.29	120.56
3	A	301	72L	CA-CB-N1	-5.74	115.16	122.41
3	A	301	72L	CE1-C15-CE2	-5.37	113.51	120.56
3	C	301	72L	O2-S1-OH	-4.85	112.35	118.87
3	C	301	72L	CD2-CE2-C18	-4.64	113.11	120.89
3	A	301	72L	C9-S1-N6	-4.49	102.69	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	72L	C10-C11-C6	-4.32	115.45	120.30
3	A	301	72L	C15-CE2-C18	-4.03	114.68	121.40
3	C	301	72L	CA-CB-N1	-3.93	117.45	122.41
3	C	301	72L	C22-C21-C20	-3.65	113.66	119.88
3	C	301	72L	N2-C2-N1	-3.54	120.89	126.18
3	C	301	72L	CD2-CG-CB	-3.45	114.52	120.34
3	A	301	72L	C11-C6-C7	-3.26	114.52	119.06
3	A	301	72L	C7-C6-N5	-3.18	110.12	120.66
3	C	301	72L	C19-C18-CE2	-3.16	116.13	121.40
3	C	301	72L	C7-C6-N5	-2.73	111.61	120.66
3	A	301	72L	C23-C18-C19	-2.65	112.39	117.56
3	A	301	72L	CA-C-N3	-2.45	106.78	111.12
3	A	301	72L	C20-C19-C18	-2.40	117.42	120.56
3	A	301	72L	C11-C10-C9	-2.14	117.20	119.49
3	A	301	72L	CD1-CG-CB	2.15	124.05	120.72
3	A	301	72L	CG-CB-CA	2.25	125.15	122.46
3	C	301	72L	C15-CE2-C18	2.35	125.33	121.40
3	C	301	72L	C23-C18-C19	2.43	122.32	117.56
3	C	301	72L	C11-C6-N5	2.45	128.79	120.66
3	C	301	72L	C21-C20-C19	2.58	123.79	120.20
3	C	301	72L	C15-CE2-CD2	2.66	121.54	118.17
3	A	301	72L	OH-S1-N6	3.21	111.24	107.25
3	C	301	72L	C2-N2-C	3.36	118.67	114.99
3	A	301	72L	N5-C2-N1	3.67	128.51	116.92
3	A	301	72L	C8-C7-C6	3.81	124.57	120.30
3	A	301	72L	CD2-CG-CB	4.05	127.18	120.34
3	A	301	72L	C7-C8-C9	4.07	123.83	119.49
3	C	301	72L	CD1-CG-CB	4.09	127.04	120.72
3	A	301	72L	CD1-CE1-C15	4.21	126.33	120.25
3	C	301	72L	C21-C22-C23	4.21	126.05	120.20
3	A	301	72L	C11-C6-N5	4.43	135.36	120.66
3	A	301	72L	CG-CB-N1	4.49	119.51	115.51
3	A	301	72L	CG-CD2-CE2	4.56	129.44	121.36
3	C	301	72L	O2-S1-N6	5.14	113.62	107.25
3	C	301	72L	C8-C7-C6	5.28	126.23	120.30
3	A	301	72L	C22-C23-C18	5.44	127.69	120.56
3	C	301	72L	CG-CB-N1	5.97	120.83	115.51
3	A	301	72L	C21-C22-C23	5.99	128.52	120.20
3	C	301	72L	C10-C9-C8	6.76	129.36	120.42
3	A	301	72L	O2-S1-N6	6.92	115.85	107.25
3	A	301	72L	O2-S1-C9	8.54	117.03	107.41
3	A	301	72L	C2-N2-C	10.22	126.20	114.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	72L	C21-C20-C19	10.66	135.01	120.20
3	A	301	72L	C10-C9-S1	12.40	138.00	119.75
3	C	301	72L	OH-S1-C9	12.74	121.77	107.41
3	A	301	72L	OH-S1-C9	15.80	125.21	107.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	72L	44	0
3	C	301	72L	17	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	295/303 (97%)	0.07	5 (1%) 73 51	27, 52, 109, 165	0
1	C	296/303 (97%)	0.46	12 (4%) 41 22	45, 88, 125, 162	0
2	B	257/260 (98%)	0.29	5 (1%) 70 48	32, 62, 92, 136	0
2	D	257/260 (98%)	0.65	27 (10%) 8 4	44, 99, 146, 182	0
All	All	1105/1126 (98%)	0.36	49 (4%) 38 21	27, 74, 130, 182	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	5.5
2	D	332	LEU	5.2
1	C	161	HIS	4.9
2	D	418	TYR	3.8
1	C	101	LEU	3.4
2	D	315	LEU	3.3
2	B	283	ASP	3.3
2	D	372	TRP	3.3
2	D	362	LEU	3.1
2	D	323	GLN	2.9
1	C	175	LEU	2.9
2	B	215	VAL	2.9
2	D	403	GLN	2.9
2	D	410	ARG	2.9
1	C	212	LEU	2.9
2	D	422	SER	2.8
2	D	412	LYS	2.8
1	A	295	HIS	2.8
1	C	99	ILE	2.8
2	D	284	ASP	2.7
2	D	360	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	411	GLU	2.5
1	C	285	PHE	2.5
1	C	290	THR	2.5
2	D	328	LYS	2.4
2	B	343	ASP	2.4
1	C	83	LEU	2.4
1	C	273	LYS	2.4
2	D	363	ALA	2.3
1	C	234	PRO	2.3
2	D	414	LYS	2.3
1	A	15	TYR	2.2
2	D	417	LYS	2.2
2	D	408	SER	2.2
2	B	206	ILE	2.2
2	D	214	LEU	2.2
1	C	97	THR	2.2
2	D	185	TYR	2.2
2	D	322	GLN	2.1
1	A	40	GLU	2.1
2	D	321	HIS	2.1
2	D	336	LEU	2.1
2	D	384	LEU	2.0
2	D	178	TYR	2.0
1	C	158	THR	2.0
2	B	175	VAL	2.0
1	A	73	GLU	2.0
2	D	366	THR	2.0
2	D	334	MET	2.0

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. 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
1	TPO	C	160	11/12	0.97	0.19	-	64,81,104,110	0
1	TPO	A	160	11/12	0.99	0.17	-	38,39,55,59	0

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(\AA^2)	Q<0.9
3	72L	A	301	32/32	0.76	0.60	7.39	171,187,204,212	0
3	72L	C	301	32/32	0.64	0.62	6.30	207,221,241,247	0

6.5 Other polymers [i](#)

There are no such residues in this entry.