



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:30 PM GMT

PDB ID : 4CFV  
Title : Structure-based design of C8-substituted O6-cyclohexylmethoxyguanine CDK1 and 2 inhibitors.  
Authors : Carbain, B.; Paterson, D.J.; Anscombe, E.; Campbell, A.; Cano, C.; Echaliér, A.; Endicott, J.; Golding, B.T.; Haggerty, K.; Hardcastle, I.R.; Jewsbury, P.; Newell, D.R.; Noble, M.E.M.; Roche, C.; Wang, L.Z.; Griffin, R.  
Deposited on : 2013-11-19  
Resolution : 2.00 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

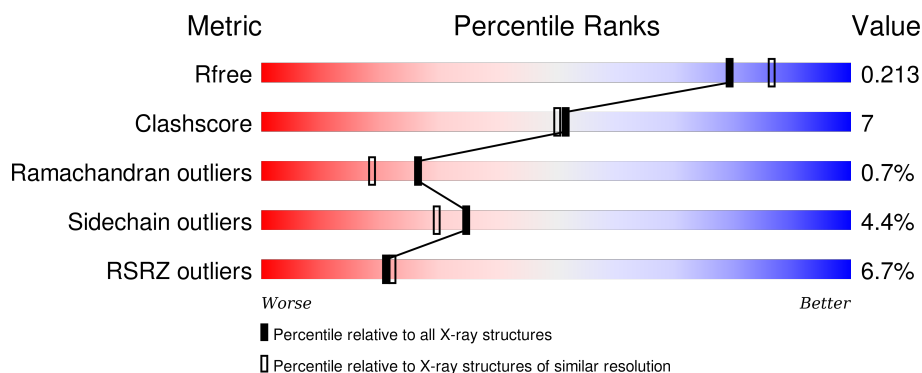
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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  $\geq 3$ , 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>7%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• •</div> </div> </div>
1	C	303	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>• 13%</div> </div> </div>
2	B	262	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>•</div> </div> </div>
2	D	262	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9640 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	301	Total	C	N	O	P	S	0	9	0
			2480	1608	421	441	1	9			
1	C	265	Total	C	N	O	P	S	0	5	0
			2169	1408	369	384	1	7			

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	PRO	-	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	PRO	-	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	262	Total	C	N	O	S		0	5	0
			2143	1388	349	396	10				
2	D	262	Total	C	N	O	S		0	3	0
			2130	1378	346	396	10				

There are 16 discrepancies between the modelled and reference sequences:

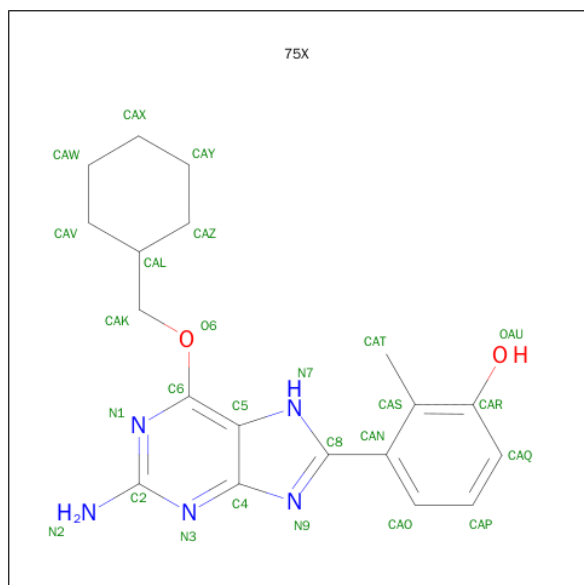
Chain	Residue	Modelled	Actual	Comment	Reference
B	171	GLY	-	EXPRESSION TAG	UNP P20248
B	311	ILE	VAL	CONFLICT	UNP P20248

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Chain	Residue	Modelled	Actual	Comment	Reference
B	357	ALA	GLY	CONFLICT	UNP P20248
B	377	VAL	ILE	CONFLICT	UNP P20248
B	378	GLN	ARG	CONFLICT	UNP P20248
B	386	THR	SER	CONFLICT	UNP P20248
B	392	LEU	MET	CONFLICT	UNP P20248
B	400	ARG	LYS	CONFLICT	UNP P20248
D	171	GLY	-	EXPRESSION TAG	UNP P20248
D	311	ILE	VAL	CONFLICT	UNP P20248
D	357	ALA	GLY	CONFLICT	UNP P20248
D	377	VAL	ILE	CONFLICT	UNP P20248
D	378	GLN	ARG	CONFLICT	UNP P20248
D	386	THR	SER	CONFLICT	UNP P20248
D	392	LEU	MET	CONFLICT	UNP P20248
D	400	ARG	LYS	CONFLICT	UNP P20248

- Molecule 3 is 3-[2-AMINO-6-(CYCLOHEXYLMETHOXY)-7H-PURIN-8-YL]-2-METHYLPHENOL (three-letter code: 75X) (formula: C<sub>19</sub>H<sub>23</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	19	5	2		
3	C	1	Total	C	N	O	0	0
			26	19	5	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

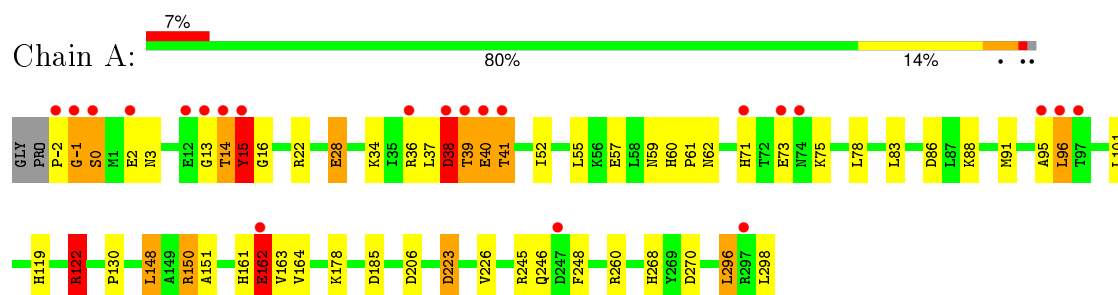
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	227	Total O 227 227	0	0
5	B	170	Total O 170 170	0	0
5	C	142	Total O 142 142	0	0
5	D	123	Total O 123 123	0	0

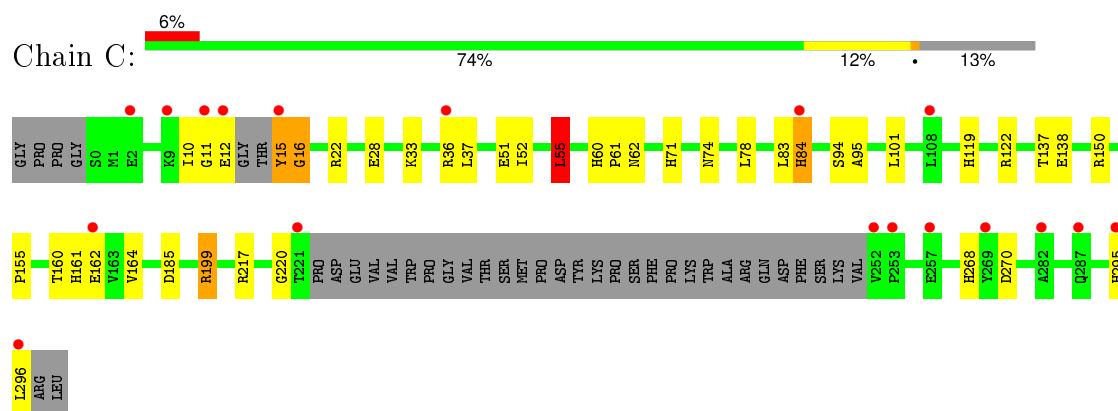
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

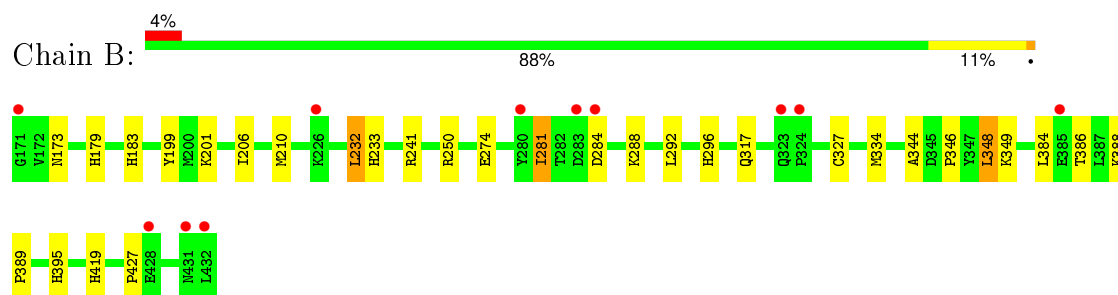
#### • Molecule 1: CYCLIN-DEPENDENT KINASE 2



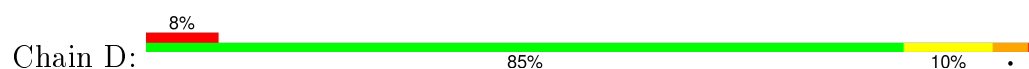
#### • Molecule 1: CYCLIN-DEPENDENT KINASE 2

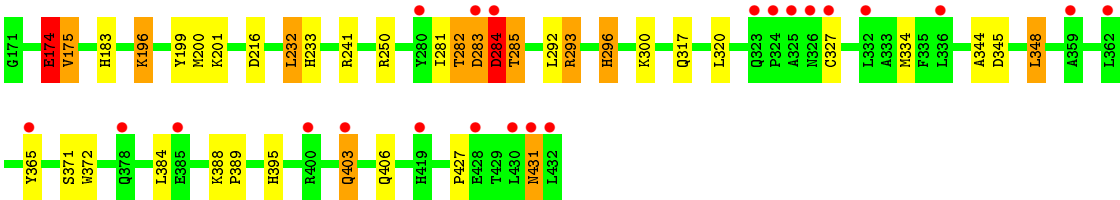


#### • Molecule 2: CYCLIN-A2



#### • Molecule 2: CYCLIN-A2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.07Å 133.91Å 147.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.00 19.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.87-2.00) 98.8 (19.87-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.178 , 0.205 0.185 , 0.213	Depositor DCC
$R_{free}$ test set	4918 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 98559 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: TPO, MG, 75X

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	1.07	4/2550 (0.2%)	1.15	18/3458 (0.5%)
1	C	0.96	2/2219 (0.1%)	1.08	4/3002 (0.1%)
2	B	0.98	0/2206	1.02	5/2998 (0.2%)
2	D	0.92	0/2186	1.04	13/2972 (0.4%)
All	All	0.99	6/9161 (0.1%)	1.07	40/12430 (0.3%)

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	4
1	C	0	1
2	D	0	2
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	GLU	CD-OE1	6.29	1.32	1.25
1	C	16	GLY	N-CA	5.77	1.54	1.46
1	A	162	GLU	C-O	5.59	1.33	1.23
1	C	138	GLU	CD-OE1	5.46	1.31	1.25
1	A	28	GLU	CD-OE2	-5.19	1.20	1.25
1	A	-1	GLY	N-CA	5.05	1.53	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ARG	NE-CZ-NH2	-16.78	111.91	120.30
1	C	199	ARG	NE-CZ-NH1	14.70	127.65	120.30
2	B	334	MET	CG-SD-CE	-9.79	84.55	100.20
2	D	250	ARG	NE-CZ-NH2	-9.40	115.60	120.30
2	D	250	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	A	245	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	38	ASP	N-CA-C	-8.22	88.81	111.00
1	A	206[A]	ASP	CB-CG-OD1	-8.13	110.98	118.30
1	A	206[B]	ASP	CB-CG-OD1	-8.13	110.98	118.30
2	D	334	MET	CG-SD-CE	-8.05	87.32	100.20
2	B	241	ARG	NE-CZ-NH2	-7.68	116.46	120.30
2	B	241	ARG	NE-CZ-NH1	7.64	124.12	120.30
2	D	175	VAL	N-CA-C	-7.58	90.53	111.00
2	D	241	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	14	THR	N-CA-C	6.48	128.49	111.00
1	A	162	GLU	CB-CA-C	6.21	122.82	110.40
1	C	199	ARG	CD-NE-CZ	6.20	132.28	123.60
2	D	174	GLU	CA-C-N	6.18	130.80	117.20
1	A	148	LEU	CB-CG-CD1	5.99	121.18	111.00
2	D	403	GLN	N-CA-CB	5.97	121.35	110.60
1	C	55	LEU	CB-CG-CD1	5.96	121.14	111.00
1	A	122[A]	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	122[B]	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	86	ASP	CB-CG-OD1	5.78	123.50	118.30
2	D	241	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	B	232	LEU	CB-CG-CD2	5.74	120.76	111.00
2	D	284	ASP	CB-CG-OD1	5.62	123.36	118.30
2	D	174	GLU	N-CA-C	5.55	126.00	111.00
1	A	15[A]	TYR	N-CA-C	5.55	125.99	111.00
1	A	15[B]	TYR	N-CA-C	5.55	125.99	111.00
1	A	296	LEU	CB-CG-CD1	5.52	120.39	111.00
1	A	91	MET	CG-SD-CE	5.44	108.91	100.20
2	D	174	GLU	C-N-CA	5.43	135.27	121.70
2	D	232	LEU	CB-CG-CD2	5.40	120.18	111.00
1	A	162	GLU	C-N-CA	5.30	134.96	121.70
1	A	150	ARG	CA-CB-CG	5.29	125.05	113.40
1	A	223	ASP	CB-CG-OD1	5.13	122.92	118.30
2	B	281	ILE	N-CA-CB	5.07	122.45	110.80
2	D	345	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	14	THR	CA-C-N	5.05	128.30	117.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	THR	Peptide
1	A	162	GLU	Peptide
1	A	37	LEU	Peptide
1	A	40	GLU	Peptide
1	C	220	GLY	Peptide
2	D	174	GLU	Peptide
2	D	282	THR	Peptide

## 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	2480	0	2527	48	0
1	C	2169	0	2222	35	0
2	B	2143	0	2162	25	0
2	D	2130	0	2142	25	0
3	A	26	0	23	1	0
3	C	26	0	22	1	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
5	A	227	0	0	16	2
5	B	170	0	0	9	0
5	C	142	0	0	7	1
5	D	123	0	0	5	0
All	All	9640	0	9098	123	2

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.

All (123) 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:122[B]:ARG:NH1	5:A:2092:HOH:O	1.95	0.98
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.83	0.96
1:A:95:ALA:O	1:A:96:LEU:HB2	1.67	0.95
1:C:71:HIS:HD2	2:D:296:HIS:HE1	1.00	0.93
1:A:22[B]:ARG:NH1	5:A:2016:HOH:O	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:282:THR:O	2:D:285:THR:OG1	1.91	0.87
1:C:71:HIS:CD2	2:D:296:HIS:HE1	1.90	0.86
1:C:160:TPO:CG2	1:C:162[B]:GLU:HG3	2.06	0.86
1:A:161:HIS:O	1:A:162:GLU:C	2.15	0.84
1:A:260:ARG:HD3	5:A:2191:HOH:O	1.77	0.83
1:C:160:TPO:HG23	1:C:162[B]:GLU:HG3	1.60	0.83
1:C:60:HIS:HD2	1:C:62:ASN:H	1.29	0.81
2:B:173[B]:ASN:ND2	5:B:2016:HOH:O	1.97	0.79
1:A:60:HIS:HD2	1:A:62:ASN:H	1.30	0.78
1:A:161:HIS:HD2	5:A:2045:HOH:O	1.68	0.77
1:C:84[A]:HIS:NE2	1:C:296:LEU:HD13	2.02	0.75
1:A:57:GLU:O	5:A:2051:HOH:O	2.04	0.75
2:D:201:LYS:NZ	5:D:2035:HOH:O	2.21	0.73
1:A:60:HIS:CD2	1:A:62:ASN:H	2.07	0.72
1:C:15[A]:TYR:CD1	1:C:15[A]:TYR:N	2.57	0.72
1:A:59[A]:ASN:ND2	5:A:2055:HOH:O	2.22	0.71
1:C:84[A]:HIS:NE2	1:C:296:LEU:CD1	2.53	0.71
1:A:161:HIS:HE1	5:A:2130:HOH:O	1.71	0.71
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.56	0.71
1:C:60:HIS:CD2	1:C:62:ASN:H	2.09	0.70
1:A:246:GLN:O	5:A:2162:HOH:O	2.11	0.69
2:D:327:CYS:SG	5:D:2099:HOH:O	2.50	0.68
1:C:74:ASN:ND2	5:C:2025:HOH:O	2.24	0.67
2:B:210:MET:CE	2:B:250:ARG:HB2	2.25	0.66
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.74	0.65
1:A:-1:GLY:HA2	1:A:0:SER:HB2	1.81	0.62
1:C:95:ALA:HA	1:C:199:ARG:HD2	1.81	0.62
1:C:11:GLY:O	1:C:12:GLU:HG3	2.00	0.62
1:C:10:ILE:O	1:C:10:ILE:CG2	2.47	0.62
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.81	0.61
1:A:178:LYS:HE3	5:A:2125:HOH:O	2.01	0.61
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.83	0.61
2:B:296:HIS:HD2	5:B:2100:HOH:O	1.85	0.59
2:B:210:MET:HE1	2:B:250:ARG:CB	2.33	0.59
1:C:10:ILE:O	1:C:10:ILE:HG22	2.03	0.59
2:B:183:HIS:HD2	5:B:2029:HOH:O	1.85	0.59
2:D:372:TRP:HB3	2:D:384:LEU:HD11	1.85	0.59
1:A:28:GLU:OE2	5:A:2023:HOH:O	2.17	0.58
1:C:119:HIS:HD2	5:C:2076:HOH:O	1.84	0.58
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.85	0.58
1:C:161:HIS:HD2	5:C:2039:HOH:O	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:HIS:HD2	5:B:2109:HOH:O	1.88	0.55
2:B:395:HIS:HE1	2:B:427:PRO:O	1.90	0.55
2:B:179[A]:HIS:CE1	5:B:2022:HOH:O	2.59	0.54
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.71	0.54
1:C:15[B]:TYR:CE2	1:C:36:ARG:HB2	2.43	0.53
2:D:200:MET:HB2	5:D:2030:HOH:O	2.07	0.53
1:A:39:THR:O	1:A:40:GLU:HB3	2.07	0.53
1:A:41:THR:HB	2:B:288:LYS:NZ	2.23	0.53
1:A:119:HIS:HD2	5:A:2090:HOH:O	1.91	0.53
1:A:268:HIS:HD2	1:A:270:ASP:H	1.56	0.53
5:A:2035:HOH:O	2:B:274:GLU:HG2	2.09	0.53
1:A:3:ASN:OD1	2:D:293:ARG:NH1	2.41	0.53
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.91	0.53
2:B:386:THR:HB	5:B:2146:HOH:O	2.09	0.53
1:A:122[B]:ARG:CZ	1:A:151:ALA:HB1	2.39	0.52
1:A:38:ASP:CG	1:A:38:ASP:O	2.47	0.52
1:A:13:GLY:HA3	5:A:2009:HOH:O	2.10	0.51
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.94	0.51
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.93	0.51
1:A:161:HIS:HB3	5:A:2129:HOH:O	2.11	0.51
1:A:15[B]:TYR:CB	1:A:16:GLY:HA2	2.41	0.50
1:A:38:ASP:O	1:A:40:GLU:N	2.44	0.50
1:A:60:HIS:HE1	5:A:2014:HOH:O	1.94	0.50
2:D:395:HIS:HE1	2:D:427:PRO:O	1.94	0.49
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.95	0.49
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.47	0.49
1:A:248:PHE:O	5:A:2190:HOH:O	2.19	0.48
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.95	0.48
1:A:15[B]:TYR:CB	1:A:16:GLY:CA	2.91	0.48
1:A:39:THR:O	1:A:40:GLU:CB	2.61	0.48
2:B:206:ILE:HG22	2:B:210:MET:HE1	1.95	0.48
1:C:94:SER:O	1:C:199:ARG:HD3	2.15	0.47
1:C:217:ARG:HD2	5:C:2129:HOH:O	2.14	0.47
1:C:268:HIS:HD2	1:C:270:ASP:H	1.63	0.47
1:A:2[B]:GLU:HG3	2:D:293:ARG:HH22	1.78	0.47
1:A:223:ASP:H	1:A:226:VAL:HG12	1.79	0.47
1:C:137:THR:HA	1:C:296:LEU:HD12	1.97	0.47
1:C:155:PRO:HG3	2:D:320:LEU:HD21	1.96	0.47
1:C:12:GLU:HG2	1:C:16:GLY:O	2.14	0.47
3:C:1297:75X:HAX	5:C:2085:HOH:O	2.15	0.47
1:C:295:HIS:CD2	1:C:295:HIS:H	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:THR:CB	5:B:2146:HOH:O	2.64	0.46
1:A:83:LEU:O	3:A:1299:75X:N9	2.48	0.46
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.51	0.46
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.84	0.46
2:B:233:HIS:HE1	5:B:2110:HOH:O	1.99	0.44
1:A:15[B]:TYR:HB3	1:A:16:GLY:CA	2.47	0.44
5:C:2054:HOH:O	2:D:296:HIS:HD2	1.99	0.44
1:A:161:HIS:O	1:A:162:GLU:O	2.36	0.44
1:C:84[A]:HIS:NE2	1:C:296:LEU:HD11	2.30	0.44
1:C:84[A]:HIS:CE1	1:C:296:LEU:HD13	2.52	0.44
2:B:284:ASP:HB2	5:B:2094:HOH:O	2.17	0.43
2:B:388:LYS:HB3	2:B:389:PRO:HD3	2.00	0.43
2:D:216:ASP:HB2	2:D:406:GLN:HG2	1.99	0.43
1:A:41:THR:HB	2:B:288:LYS:HZ3	1.82	0.43
1:A:95:ALA:O	1:A:96:LEU:CB	2.43	0.43
1:C:51:GLU:O	1:C:55:LEU:HB2	2.19	0.43
2:D:283[A]:ASP:O	2:D:284:ASP:HB2	2.18	0.42
2:D:196:LYS:HG2	2:D:199:TYR:HB3	2.01	0.42
2:D:365:TYR:OH	2:D:431:ASN:OD1	2.35	0.42
1:C:11:GLY:C	1:C:12:GLU:HG3	2.39	0.42
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.54	0.42
1:C:15[B]:TYR:HA	1:C:16:GLY:HA2	1.79	0.42
2:B:210:MET:HB3	2:B:210:MET:HE2	1.77	0.42
1:C:28:GLU:OE2	5:C:2015:HOH:O	2.21	0.42
1:A:88:LYS:HB2	1:A:130:PRO:HB2	2.01	0.42
1:A:-1:GLY:CA	1:A:0:SER:HB2	2.49	0.42
1:A:15[B]:TYR:CE2	1:A:36:ARG:HD2	2.55	0.42
2:D:233:HIS:HE1	5:D:2091:HOH:O	2.01	0.42
2:D:388:LYS:HB3	2:D:389:PRO:HD3	2.02	0.41
2:B:346:PRO:O	2:B:349:LYS:HG2	2.21	0.41
2:D:371:SER:O	2:D:372:TRP:C	2.58	0.41
2:B:327:CYS:HB3	2:B:419:HIS:CE1	2.55	0.41
1:A:55:LEU:HA	1:A:55:LEU:HD23	1.92	0.41
1:A:38:ASP:O	1:A:39:THR:C	2.60	0.40
2:D:233:HIS:HD2	5:D:2090:HOH:O	2.04	0.40
1:A:-2:PRO:O	2:D:300:LYS:HD3	2.22	0.40

All (2) 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)
5:A:2160:HOH:O	5:A:2214:HOH:O[4_555]	2.02	0.18
5:A:2224:HOH:O	5:C:2126:HOH:O[3_454]	2.12	0.08

## 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	307/303 (101%)	293 (95%)	10 (3%)	4 (1%)	15	7
1	C	262/303 (86%)	255 (97%)	6 (2%)	1 (0%)	39	33
2	B	265/262 (101%)	262 (99%)	3 (1%)	0	100	100
2	D	263/262 (100%)	256 (97%)	3 (1%)	4 (2%)	13	5
All	All	1097/1130 (97%)	1066 (97%)	22 (2%)	9 (1%)	26	15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	96	LEU
1	A	164	VAL
1	C	164	VAL
2	D	284	ASP
1	A	162	GLU
2	D	431	ASN
2	D	283[A]	ASP
2	D	283[B]	ASP

### 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	273/265 (103%)	257 (94%)	16 (6%)	24	18
1	C	237/265 (89%)	224 (94%)	13 (6%)	27	21
2	B	239/235 (102%)	232 (97%)	7 (3%)	50	49
2	D	237/235 (101%)	226 (95%)	11 (5%)	33	28
All	All	986/1000 (99%)	939 (95%)	47 (5%)	35	26

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15[A]	TYR
1	A	15[B]	TYR
1	A	34	LYS
1	A	38	ASP
1	A	39	THR
1	A	41	THR
1	A	73	GLU
1	A	75	LYS
1	A	101	LEU
1	A	122[A]	ARG
1	A	122[B]	ARG
1	A	148	LEU
1	A	150	ARG
1	A	163	VAL
1	A	296	LEU
1	A	298	LEU
2	B	199	TYR
2	B	201	LYS
2	B	232	LEU
2	B	281	ILE
2	B	292	LEU
2	B	348	LEU
2	B	384	LEU
1	C	15[A]	TYR
1	C	15[B]	TYR
1	C	22[A]	ARG
1	C	22[B]	ARG
1	C	33	LYS
1	C	37	LEU
1	C	55	LEU
1	C	83	LEU

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Mol	Chain	Res	Type
1	C	84[A]	HIS
1	C	84[B]	HIS
1	C	101	LEU
1	C	122	ARG
1	C	150	ARG
2	D	174	GLU
2	D	175	VAL
2	D	196	LYS
2	D	232	LEU
2	D	281	ILE
2	D	285	THR
2	D	292	LEU
2	D	293	ARG
2	D	296	HIS
2	D	348	LEU
2	D	403	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	119	HIS
1	A	161	HIS
1	A	268	HIS
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	317	GLN
2	B	395	HIS
2	B	403	GLN
2	B	431	ASN
1	C	60	HIS
1	C	71	HIS
1	C	119	HIS
1	C	161	HIS
1	C	268	HIS
1	C	295	HIS
2	D	173	ASN
2	D	183	HIS
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS

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Mol	Chain	Res	Type
2	D	317	GLN
2	D	395	HIS
2	D	396	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	TPO	A	160	1	8,10,11	0.91	0	7,14,16	1.37	0
1	TPO	C	160	1	8,10,11	0.97	0	7,14,16	1.45	2 (28%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O-C-CA	-2.34	119.25	125.44
1	C	160	TPO	O3P-P-O2P	2.10	115.39	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	160	TPO	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are 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	$\# Z  > 2$
3	75X	A	1299	-	28,29,29	1.96	6 (21%)	29,41,41	2.33	7 (24%)
3	75X	C	1297	-	28,29,29	2.16	9 (32%)	29,41,41	2.85	14 (48%)

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	75X	A	1299	-	-	0/9/17/17	0/4/4/4
3	75X	C	1297	-	-	0/9/17/17	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1299	75X	CAN-C8	-5.39	1.37	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1297	75X	CAN-C8	-5.35	1.37	1.48
3	A	1299	75X	CAT-CAS	-4.74	1.42	1.51
3	C	1297	75X	CAT-CAS	-3.94	1.43	1.51
3	C	1297	75X	C2-N2	-2.69	1.28	1.34
3	A	1299	75X	C5-C4	-2.01	1.36	1.40
3	C	1297	75X	C8-N7	2.06	1.38	1.35
3	C	1297	75X	C6-N1	2.45	1.36	1.31
3	C	1297	75X	CAO-CAN	2.76	1.44	1.39
3	A	1299	75X	CAY-CAZ	2.84	1.60	1.53
3	C	1297	75X	CAR-CAS	2.87	1.44	1.40
3	A	1299	75X	CAO-CAN	3.00	1.45	1.39
3	A	1299	75X	C6-N1	3.00	1.37	1.31
3	C	1297	75X	CAY-CAZ	3.29	1.62	1.53
3	C	1297	75X	O6-C6	4.76	1.38	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1297	75X	O6-CAK-CAL	-5.97	94.19	107.97
3	A	1299	75X	CAY-CAZ-CAL	-5.78	102.90	112.22
3	C	1297	75X	CAW-CAV-CAL	-5.57	103.24	112.22
3	C	1297	75X	CAY-CAZ-CAL	-5.40	103.51	112.22
3	A	1299	75X	O6-CAK-CAL	-5.27	95.81	107.97
3	A	1299	75X	N3-C2-N1	-3.99	121.37	127.44
3	C	1297	75X	N3-C2-N1	-3.46	122.17	127.44
3	A	1299	75X	CAW-CAV-CAL	-3.44	106.66	112.22
3	C	1297	75X	N2-C2-N1	-2.90	112.39	117.20
3	C	1297	75X	CAP-CAQ-CAR	-2.89	116.32	120.04
3	C	1297	75X	CAO-CAN-CAS	-2.88	116.96	120.06
3	C	1297	75X	CAN-C8-N9	-2.65	120.53	123.78
3	C	1297	75X	O6-C6-C5	2.20	118.51	115.07
3	A	1299	75X	C2-N1-C6	2.21	119.07	116.03
3	C	1297	75X	CAQ-CAR-CAS	2.71	126.62	121.93
3	A	1299	75X	N2-C2-N3	2.80	123.17	117.80
3	C	1297	75X	CAT-CAS-CAR	2.81	124.36	120.53
3	C	1297	75X	CAP-CAO-CAN	2.82	125.24	120.33
3	C	1297	75X	N2-C2-N3	3.95	125.37	117.80
3	C	1297	75X	CAN-C8-N7	5.43	130.45	123.78
3	A	1299	75X	CAN-C8-N7	5.93	131.07	123.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1299	75X	1	0
3	C	1297	75X	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	300/303 (99%)	0.15	22 (7%)	18 19	14, 24, 51, 76	0
1	C	264/303 (87%)	0.23	18 (6%)	20 22	21, 32, 49, 62	0
2	B	262/262 (100%)	-0.03	11 (4%)	40 41	17, 27, 41, 56	0
2	D	262/262 (100%)	0.31	22 (8%)	14 14	18, 35, 68, 94	0
All	All	1088/1130 (96%)	0.17	73 (6%)	21 22	14, 29, 56, 94	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	7.9
2	D	283[A]	ASP	6.7
1	A	15[A]	TYR	6.6
1	A	96	LEU	6.6
1	A	14	THR	6.3
1	C	15[A]	TYR	6.0
1	C	253	PRO	5.8
2	D	431	ASN	5.7
1	A	41	THR	5.6
2	D	432	LEU	5.4
1	C	221	THR	4.8
2	B	284	ASP	4.5
1	A	38	ASP	4.5
1	A	13	GLY	4.2
2	B	283[A]	ASP	4.2
1	C	295	HIS	4.1
2	B	323	GLN	4.1
1	C	12	GLU	4.0
1	A	40	GLU	3.9
1	A	36	ARG	3.8
2	B	171	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	71	HIS	3.8
1	C	296	LEU	3.7
1	A	162	GLU	3.7
1	A	-2	PRO	3.6
2	D	323	GLN	3.5
2	D	430	LEU	3.5
1	A	73	GLU	3.5
1	A	0	SER	3.4
2	D	284	ASP	3.4
1	C	287	GLN	3.2
1	C	36	ARG	3.2
2	D	325	ALA	3.1
2	B	280	TYR	3.1
2	D	365	TYR	3.1
2	D	378	GLN	3.1
2	D	428	GLU	3.1
2	D	280	TYR	3.0
1	A	-1	GLY	2.9
1	C	269	TYR	2.9
1	C	9	LYS	2.9
2	D	332	LEU	2.7
1	A	2[A]	GLU	2.7
1	A	95	ALA	2.7
2	D	359	ALA	2.7
1	C	108	LEU	2.6
1	A	97	THR	2.6
1	A	74	ASN	2.5
1	C	282	ALA	2.5
2	B	428	GLU	2.5
2	D	419	HIS	2.5
1	C	162[A]	GLU	2.5
2	D	324	PRO	2.5
2	D	336	LEU	2.4
2	D	362	LEU	2.4
2	D	385	GLU	2.4
2	D	400	ARG	2.3
2	D	403	GLN	2.3
2	B	385[A]	GLU	2.3
2	B	432	LEU	2.3
1	C	252	VAL	2.3
1	C	257	GLU	2.3
2	B	324	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	327	CYS	2.2
1	C	11	GLY	2.1
1	C	84[A]	HIS	2.1
2	B	226	LYS	2.1
2	D	326	ASN	2.1
1	A	12	GLU	2.0
1	A	247	ASP	2.0
1	C	2	GLU	2.0
1	A	297	ARG	2.0
2	B	431	ASN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	TPO	A	160	11/12	0.98	0.06	-	20,22,23,23	0
1	TPO	C	160	11/12	0.98	0.06	-	24,27,29,30	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	75X	A	1299	26/26	0.90	0.20	1.50	28,36,43,44	0
4	MG	D	1434	1/1	0.98	0.20	1.22	32,32,32,32	0
3	75X	C	1297	26/26	0.85	0.21	0.67	28,40,44,46	0

*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	B	1433	1/1	0.97	0.10	0.03	32,32,32,32	0
4	MG	B	1434	1/1	0.98	0.12	0.01	32,32,32,32	0
4	MG	D	1433	1/1	0.98	0.08	-1.26	34,34,34,34	0

## 6.5 Other polymers

There are no such residues in this entry.