



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:55 AM GMT

PDB ID : 1H26  
Title : CDK2/CYCLIN A IN COMPLEX WITH AN 11-RESIDUE RECRUITMENT PEPTIDE FROM P53  
Authors : Tews, I.; Cheng, K.Y.; Lowe, E.D.; Noble, M.E.M.; Brown, N.R.; Gul, S.; Gamblin, S.; Johnson, L.N.  
Deposited on : 2002-07-31  
Resolution : 2.24 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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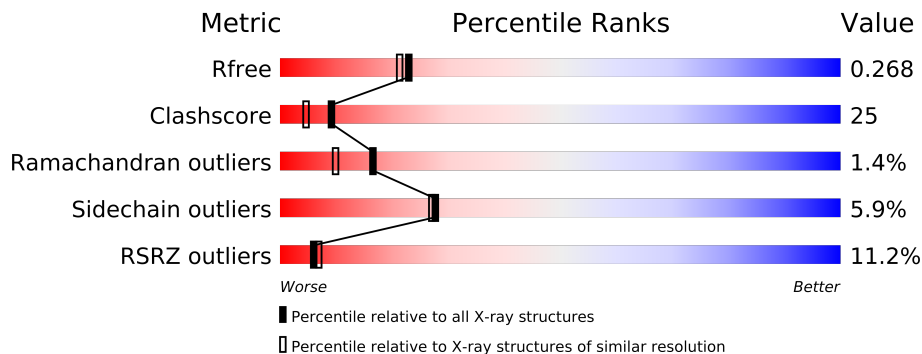
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


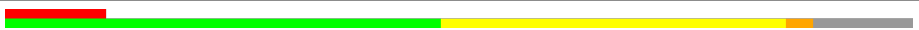

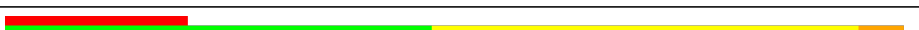
The reported resolution of this entry is 2.24 Å.

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))
$R_{free}$	66092	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (2.26-2.22)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	303	
1	C	303	
2	B	259	
2	D	259	
3	E	11	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8981 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	P	S	9	0	1
			2389	1550	405	425	1	8			
1	C	269	Total	C	N	O	P	S	0	0	1
			2149	1392	367	382	1	7			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S		0	0	0
			2084	1350	339	384	11				
2	D	258	Total	C	N	O	S		0	0	0
			2084	1350	339	384	11				

- Molecule 3 is a protein called CELLULAR TUMOR ANTIGEN P53.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	S		0	0	0
			82	53	17	11	1				

- Molecule 4 is water.

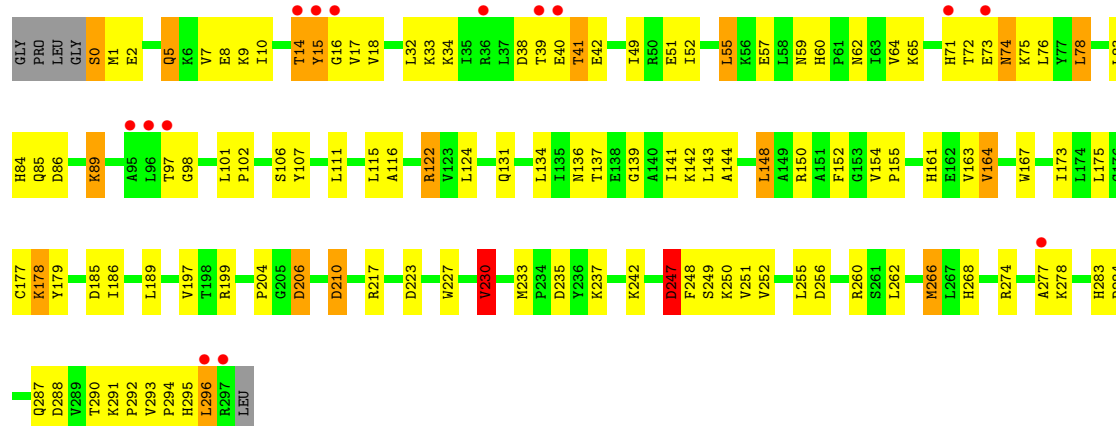
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	66	Total	O	0	0
			66	66		
4	C	19	Total	O	0	0
			19	19		
4	D	21	Total	O	0	0
			21	21		

### 3 Residue-property plots

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.

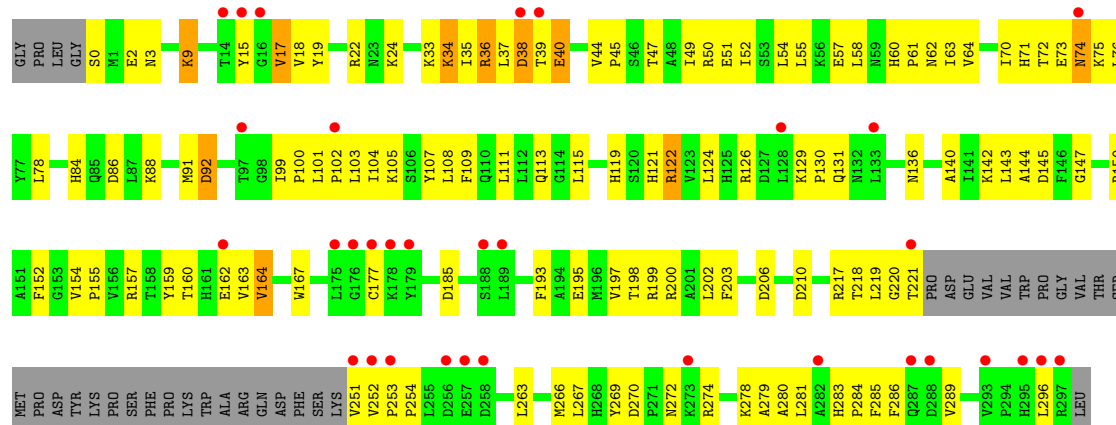
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A: 



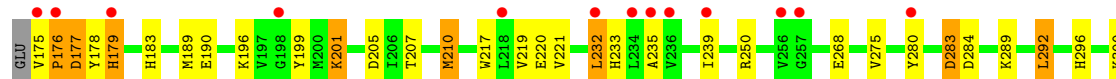
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

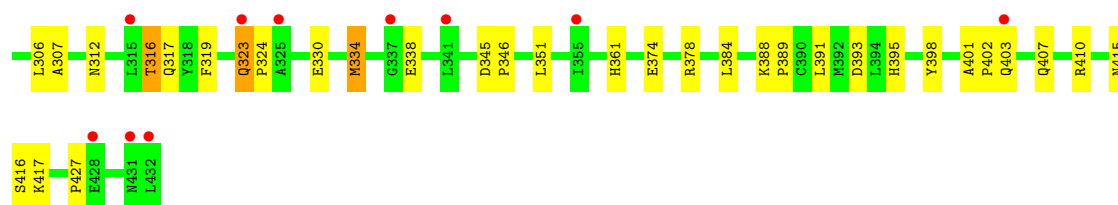
Chain C: 



#### • Molecule 2: CYCLIN A2

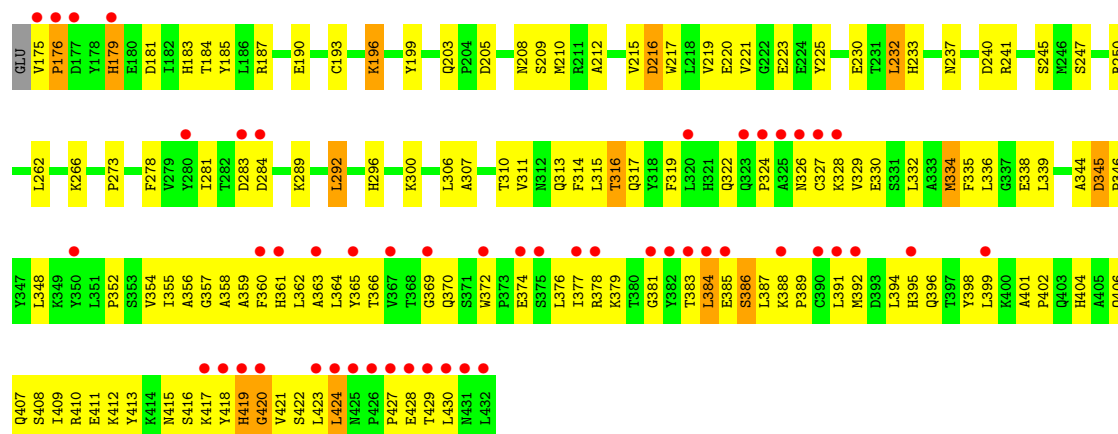
Chain B: 





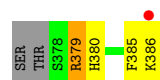
• Molecule 2: CYCLIN A2

Chain D:



• Molecule 3: CELLULAR TUMOR ANTIGEN P53

Chain E:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.67Å 134.03Å 147.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.24 29.87 – 2.24	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.88-2.24) 96.5 (29.87-2.24)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.216 , 0.268 0.232 , 0.268	Depositor DCC
$R_{free}$ test set	3460 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 33.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 68281 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8981	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	1.08	3/2439 (0.1%)	1.06	15/3310 (0.5%)
1	C	0.80	0/2186	0.90	5/2961 (0.2%)
2	B	0.98	4/2134 (0.2%)	0.88	8/2897 (0.3%)
2	D	0.86	0/2134	0.93	8/2897 (0.3%)
3	E	0.78	0/83	0.74	0/104
All	All	0.94	7/8976 (0.1%)	0.95	36/12169 (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	1
1	C	0	3
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	MET	SD-CE	-10.93	1.16	1.77
1	A	89	LYS	C-N	-8.29	1.15	1.34
1	A	116	ALA	CA-CB	5.64	1.64	1.52
2	B	210	MET	SD-CE	-5.60	1.46	1.77
2	B	268	GLU	CD-OE2	-5.53	1.19	1.25
2	B	338	GLU	CD-OE2	-5.38	1.19	1.25
2	B	398	TYR	CD2-CE2	-5.16	1.31	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LYS	C-N-CA	9.83	146.27	121.70
1	A	89	LYS	O-C-N	-8.60	108.93	122.70
2	B	378	ARG	NE-CZ-NH2	7.77	124.19	120.30
1	A	122	ARG	NE-CZ-NH1	7.43	124.01	120.30
2	D	181	ASP	CB-CG-OD2	7.18	124.76	118.30
1	A	247	ASP	CB-CG-OD2	7.08	124.68	118.30
1	A	274	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	C	210	ASP	CB-CG-OD2	6.93	124.54	118.30
2	B	177	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	230	VAL	CB-CA-C	-6.83	98.43	111.40
1	C	206	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	223	ASP	CB-CG-OD2	6.64	124.27	118.30
1	A	256	ASP	CB-CG-OD2	6.50	124.15	118.30
1	C	92	ASP	CB-CG-OD2	6.46	124.11	118.30
2	D	283	ASP	CB-CG-OD2	6.08	123.78	118.30
2	B	205	ASP	CB-CG-OD2	6.05	123.74	118.30
1	C	206	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	A	235	ASP	CB-CG-OD2	5.98	123.68	118.30
2	D	345	ASP	CB-CG-OD2	5.91	123.62	118.30
2	D	284	ASP	CB-CG-OD2	5.79	123.52	118.30
2	B	378	ARG	NE-CZ-NH1	-5.77	117.41	120.30
1	A	288	ASP	CB-CG-OD2	5.67	123.40	118.30
2	D	216	ASP	CB-CG-OD2	5.63	123.37	118.30
2	B	283	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	284	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	210	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	89	LYS	CA-C-N	5.41	129.11	117.20
2	D	205	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	296	LEU	O-C-N	-5.37	114.11	122.70
2	B	393	ASP	CB-CG-OD2	5.35	123.11	118.30
2	D	240	ASP	CB-CG-OD1	5.21	122.99	118.30
2	B	205	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	206	ASP	CB-CG-OD2	5.14	122.93	118.30
2	D	378	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	C	86	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	38	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	SER	Peptide
1	C	160	TPO	Mainchain

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Mol	Chain	Res	Type	Group
1	C	37	LEU	Peptide
1	C	70	ILE	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2389	0	2428	137	1
1	C	2149	0	2203	150	0
2	B	2084	0	2107	72	1
2	D	2084	0	2107	131	0
3	E	82	0	92	9	0
4	A	87	0	0	10	0
4	B	66	0	0	8	0
4	C	19	0	0	1	0
4	D	21	0	0	2	0
All	All	8981	0	8937	443	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (443) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:15:TYR:HE2	1:C:47:THR:OG1	1.16	1.29
1:C:17:VAL:HG11	1:C:19:TYR:CZ	1.70	1.25
1:A:266:MET:CE	1:A:266:MET:SD	1.16	1.25
1:A:266:MET:CG	1:A:266:MET:CE	2.21	1.18
1:C:39:THR:O	2:D:292:LEU:CD2	1.90	1.18
1:C:39:THR:O	2:D:292:LEU:HD23	0.99	1.17
1:A:266:MET:HE2	1:A:266:MET:SD	1.74	1.16
1:A:266:MET:HE1	1:A:266:MET:SD	1.74	1.14
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.29	1.12
1:A:266:MET:SD	1:A:266:MET:HE3	1.74	1.08
1:C:71:HIS:CD2	2:D:296:HIS:NE2	2.27	1.03
1:C:71:HIS:NE2	2:D:296:HIS:NE2	2.07	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:60:HIS:CD2	1:C:62:ASN:H	1.79	1.01
1:C:64:VAL:HG21	1:C:144:ALA:CB	1.90	1.01
1:C:64:VAL:HG23	1:C:143:LEU:O	1.60	1.01
2:D:193:CYS:SG	4:D:2009:HOH:O	2.18	1.00
2:B:296:HIS:CD2	2:B:300:LYS:HE2	1.99	0.97
4:A:2010:HOH:O	2:B:189:MET:HE2	1.64	0.97
1:A:39:THR:HG21	2:B:289:LYS:HD2	1.46	0.96
1:C:64:VAL:CG2	1:C:144:ALA:HB2	1.97	0.95
1:C:121:HIS:O	1:C:122:ARG:HG3	1.67	0.94
1:C:15:TYR:OH	1:C:47:THR:HB	1.69	0.93
1:C:60:HIS:HD2	1:C:62:ASN:H	0.96	0.92
1:A:41:THR:HA	4:A:2008:HOH:O	1.70	0.92
1:A:177:CYS:HB2	4:A:2048:HOH:O	1.67	0.92
1:A:39:THR:HG21	2:B:289:LYS:CD	1.99	0.90
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.53	0.89
1:A:39:THR:HG21	2:B:289:LYS:CE	2.01	0.89
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.55	0.89
2:B:283:ASP:HB2	3:E:380:HIS:O	1.75	0.87
1:A:210:ASP:OD1	4:A:2062:HOH:O	1.91	0.87
1:A:64:VAL:HG21	1:A:144:ALA:HB2	1.57	0.86
1:C:17:VAL:CG1	1:C:19:TYR:CZ	2.58	0.86
1:A:217:ARG:NH2	4:A:2063:HOH:O	2.09	0.85
1:A:177:CYS:SG	1:A:179:TYR:O	2.35	0.85
2:D:216:ASP:OD1	2:D:408:SER:OG	1.95	0.84
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.59	0.83
1:C:15:TYR:HE2	1:C:47:THR:CB	1.92	0.83
1:A:154:VAL:O	2:B:316:THR:HG22	1.79	0.83
2:D:387:LEU:O	2:D:391:LEU:HB2	1.79	0.82
2:D:413:TYR:O	2:D:422:SER:OG	1.97	0.81
1:C:15:TYR:HD1	1:C:33:LYS:CE	1.94	0.80
1:C:15:TYR:CE2	1:C:47:THR:CB	2.64	0.80
1:C:60:HIS:HD2	1:C:62:ASN:N	1.78	0.80
1:C:71:HIS:HB3	2:D:300:LYS:NZ	1.96	0.80
2:D:175:VAL:N	2:D:179:HIS:CE1	2.51	0.79
1:C:154:VAL:O	2:D:316:THR:HG22	1.83	0.79
1:A:39:THR:CB	2:B:289:LYS:HZ1	1.97	0.78
1:A:266:MET:CG	1:A:266:MET:HE3	2.02	0.78
2:D:233:HIS:ND1	4:D:2008:HOH:O	2.15	0.78
1:A:230:VAL:HG12	1:A:233:MET:CE	2.13	0.78
1:A:154:VAL:O	2:B:316:THR:CG2	2.32	0.78
1:C:57:GLU:OE2	2:D:307:ALA:HB3	1.84	0.77
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.15	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:17:VAL:HG11	1:C:19:TYR:CE1	2.21	0.76
1:C:15:TYR:CD1	1:C:33:LYS:CE	2.70	0.75
2:D:176:PRO:HA	2:D:179:HIS:CG	2.22	0.75
1:A:85:GLN:HG3	1:A:86:ASP:H	1.52	0.75
1:A:64:VAL:HG23	1:A:143:LEU:O	1.87	0.74
1:C:251:VAL:HG12	1:C:252:VAL:HG23	1.67	0.74
1:A:227:TRP:O	1:A:230:VAL:HG22	1.87	0.74
1:A:284:PRO:O	1:A:287:GLN:HG2	1.88	0.73
1:A:42:GLU:OE1	2:B:275:VAL:HG23	1.88	0.73
1:A:39:THR:CB	2:B:289:LYS:NZ	2.52	0.73
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.24	0.73
2:D:327:CYS:HG	2:D:419:HIS:CE1	2.06	0.73
2:B:175:VAL:N	2:B:179:HIS:CE1	2.56	0.72
1:C:17:VAL:CG1	1:C:19:TYR:CE1	2.72	0.72
1:A:148:LEU:HD23	4:A:2041:HOH:O	1.89	0.72
1:A:72:THR:HG22	1:A:74:ASN:ND2	2.04	0.72
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.24	0.71
1:C:72:THR:HG22	1:C:73:GLU:N	2.06	0.71
1:A:178:LYS:HE2	1:A:179:TYR:CZ	2.25	0.71
2:D:296:HIS:CD2	2:D:300:LYS:HE2	2.26	0.71
1:C:17:VAL:HG11	1:C:19:TYR:CE2	2.26	0.71
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.21	0.71
1:A:85:GLN:HG3	1:A:86:ASP:N	2.05	0.71
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.26	0.70
1:A:39:THR:CG2	2:B:289:LYS:HD2	2.20	0.70
1:A:72:THR:CG2	1:A:74:ASN:ND2	2.54	0.70
2:D:210:MET:HE2	2:D:250:ARG:HB2	1.73	0.70
2:B:175:VAL:HG12	4:B:2008:HOH:O	1.92	0.70
2:D:415:ASN:OD1	2:D:417:LYS:N	2.25	0.70
1:A:101:LEU:N	1:A:102:PRO:CD	2.55	0.70
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.60	0.69
1:C:40:GLU:CD	1:C:40:GLU:H	1.96	0.69
1:A:17:VAL:HG12	1:A:18:VAL:N	2.07	0.69
1:A:197:VAL:HG11	1:A:252:VAL:HG12	1.75	0.68
1:C:71:HIS:NE2	2:D:296:HIS:CD2	2.60	0.68
1:C:107:TYR:O	1:C:111:LEU:HG	1.93	0.68
1:C:105:LYS:HE2	1:C:285:PHE:CZ	2.29	0.68
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.23	0.68
1:A:39:THR:HG22	1:A:40:GLU:H	1.59	0.67
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.09	0.67
1:C:154:VAL:O	2:D:316:THR:CG2	2.42	0.67
2:D:210:MET:CE	2:D:250:ARG:HB2	2.25	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.60	0.67
2:B:296:HIS:CD2	2:B:300:LYS:CE	2.76	0.67
2:D:327:CYS:SG	2:D:419:HIS:NE2	2.68	0.66
1:A:39:THR:HG21	2:B:289:LYS:NZ	2.10	0.66
1:A:60:HIS:HD2	1:A:62:ASN:H	1.44	0.66
1:C:15:TYR:CZ	1:C:47:THR:HB	2.30	0.66
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.77	0.66
1:C:71:HIS:CG	2:D:300:LYS:HZ3	2.13	0.66
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.30	0.66
1:C:15:TYR:OH	1:C:147:GLY:HA2	1.97	0.65
1:A:230:VAL:HG12	1:A:233:MET:HE3	1.78	0.65
1:C:100:PRO:O	1:C:104:ILE:HG13	1.97	0.65
1:C:51:GLU:O	1:C:55:LEU:HB2	1.96	0.65
2:D:413:TYR:C	2:D:422:SER:OG	2.35	0.65
1:A:230:VAL:CG1	1:A:233:MET:CE	2.74	0.65
1:C:197:VAL:HG11	1:C:252:VAL:HG12	1.80	0.64
2:D:190:GLU:OE1	2:D:352:PRO:HD2	1.96	0.64
1:A:5:GLN:HA	1:A:5:GLN:HE21	1.62	0.64
1:A:266:MET:HG3	1:A:266:MET:HE3	1.78	0.64
2:B:296:HIS:NE2	2:B:300:LYS:HE2	2.11	0.64
1:A:230:VAL:CG1	1:A:233:MET:HE2	2.28	0.64
2:D:327:CYS:SG	2:D:419:HIS:CD2	2.92	0.63
1:A:39:THR:HB	2:B:289:LYS:NZ	2.13	0.63
2:D:416:SER:O	2:D:419:HIS:N	2.30	0.63
1:C:15:TYR:HD1	1:C:33:LYS:HE3	1.63	0.63
1:A:16:GLY:HA3	1:A:34:LYS:O	1.99	0.62
1:A:266:MET:CE	1:A:266:MET:HG3	2.25	0.62
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.82	0.62
2:D:419:HIS:O	2:D:421:VAL:N	2.32	0.62
2:D:336:LEU:HB2	2:D:359:ALA:HB1	1.80	0.62
1:C:101:LEU:N	1:C:102:PRO:CD	2.61	0.62
2:B:233:HIS:HD2	4:B:2041:HOH:O	1.83	0.61
1:A:39:THR:HG22	1:A:40:GLU:N	2.14	0.61
1:A:293:VAL:HG13	1:A:294:PRO:HD2	1.82	0.61
2:D:423:LEU:O	2:D:424:LEU:O	2.19	0.61
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.82	0.61
2:B:178:TYR:N	4:B:2009:HOH:O	1.90	0.61
2:D:329:VAL:O	2:D:332:LEU:N	2.33	0.60
1:A:72:THR:CG2	1:A:74:ASN:HD21	2.14	0.60
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.84	0.60
1:A:51:GLU:O	1:A:55:LEU:HB2	2.01	0.60
1:A:97:THR:HG21	1:A:295:HIS:CE1	2.36	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:60:HIS:CD2	1:A:62:ASN:H	2.20	0.59
2:D:208:ASN:OD1	2:D:344:ALA:HB3	2.01	0.59
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.29	0.59
1:A:230:VAL:HG13	1:A:233:MET:HE2	1.84	0.59
2:D:355:ILE:O	2:D:356:ALA:C	2.40	0.59
1:C:121:HIS:C	1:C:122:ARG:HG3	2.21	0.59
2:B:296:HIS:NE2	2:B:300:LYS:NZ	2.50	0.59
1:C:198:THR:O	1:C:199:ARG:HB2	2.02	0.59
2:D:209:SER:O	2:D:212:ALA:HB3	2.02	0.59
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.37	0.59
1:C:71:HIS:NE2	2:D:296:HIS:CE1	2.70	0.59
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.90	0.59
2:D:262:LEU:HD11	2:D:266:LYS:HE3	1.85	0.59
1:A:249:SER:HA	1:A:260:ARG:HD3	1.84	0.58
1:A:10:ILE:HG22	1:A:10:ILE:O	2.03	0.58
2:D:334:MET:HE3	2:D:334:MET:HA	1.85	0.58
1:A:64:VAL:CG2	1:A:144:ALA:HB2	2.32	0.58
1:C:263:LEU:HD12	1:C:263:LEU:O	2.04	0.58
1:C:39:THR:HG21	2:D:289:LYS:HE3	1.85	0.58
2:B:280:TYR:CE2	3:E:380:HIS:CE1	2.92	0.58
1:A:72:THR:HG22	1:A:74:ASN:H	1.69	0.57
2:D:196:LYS:O	2:D:196:LYS:HG3	2.04	0.57
2:B:175:VAL:N	2:B:179:HIS:HE1	2.01	0.57
1:A:39:THR:CG2	2:B:289:LYS:NZ	2.68	0.57
2:B:316:THR:HG21	4:B:2045:HOH:O	2.04	0.57
2:D:360:PHE:O	2:D:361:HIS:C	2.42	0.57
1:A:85:GLN:CG	1:A:86:ASP:N	2.67	0.57
2:D:418:TYR:O	2:D:419:HIS:C	2.43	0.56
2:D:338:GLU:HG2	2:D:409:ILE:HD13	1.87	0.56
1:A:17:VAL:CG1	1:A:18:VAL:N	2.69	0.56
2:D:332:LEU:O	2:D:336:LEU:HG	2.06	0.56
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.86	0.56
1:A:18:VAL:HA	1:A:32:LEU:O	2.06	0.56
1:C:15:TYR:HD1	1:C:33:LYS:NZ	2.04	0.56
1:C:9:LYS:NZ	1:C:17:VAL:HG22	2.21	0.56
1:A:148:LEU:CD2	4:A:2041:HOH:O	2.51	0.56
1:A:101:LEU:N	1:A:102:PRO:HD3	2.21	0.56
1:A:291:LYS:HB2	4:A:2019:HOH:O	2.04	0.55
1:C:15:TYR:CE2	1:C:47:THR:HB	2.39	0.55
1:C:220:GLY:O	1:C:221:THR:C	2.43	0.55
1:A:175:LEU:HD13	1:A:233:MET:HE1	1.88	0.55
1:C:72:THR:CG2	1:C:73:GLU:N	2.70	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.87	0.55
2:B:415:ASN:OD1	2:B:417:LYS:N	2.27	0.55
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.88	0.55
2:D:418:TYR:O	2:D:420:GLY:N	2.39	0.55
2:D:196:LYS:HG2	2:D:199:TYR:HB3	1.89	0.55
1:C:71:HIS:CE1	2:D:296:HIS:CD2	2.95	0.55
2:B:296:HIS:NE2	2:B:300:LYS:CE	2.69	0.55
2:D:387:LEU:O	2:D:391:LEU:CB	2.52	0.55
2:D:410:ARG:O	2:D:411:GLU:C	2.43	0.55
2:D:175:VAL:N	2:D:179:HIS:HE1	2.01	0.54
1:C:71:HIS:CB	2:D:300:LYS:NZ	2.69	0.54
2:D:273:PRO:HB2	2:D:278:PHE:CE2	2.43	0.54
1:C:17:VAL:HG12	1:C:19:TYR:CE1	2.42	0.54
2:D:335:PHE:CE2	2:D:339:LEU:HD11	2.42	0.54
1:C:115:LEU:HD11	1:C:119:HIS:CE1	2.42	0.54
2:B:296:HIS:HD2	2:B:300:LYS:HE2	1.61	0.54
2:D:203:GLN:OE1	2:D:247:SER:HA	2.08	0.54
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.43	0.54
1:A:71:HIS:ND1	2:B:300:LYS:NZ	2.56	0.54
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.42	0.53
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.43	0.53
1:C:18:VAL:HG22	1:C:33:LYS:HG3	1.90	0.53
1:C:71:HIS:HB3	2:D:300:LYS:HZ3	1.73	0.53
2:D:395:HIS:ND1	2:D:430:LEU:HD21	2.23	0.53
1:C:105:LYS:HE2	1:C:285:PHE:CE2	2.43	0.53
2:D:383:THR:O	2:D:385:GLU:N	2.42	0.53
2:D:361:HIS:O	2:D:362:LEU:C	2.47	0.53
2:D:175:VAL:C	2:D:179:HIS:CE1	2.82	0.53
1:A:197:VAL:CG1	1:A:252:VAL:CG1	2.84	0.53
1:C:126:ARG:O	1:C:164:VAL:HG22	2.09	0.53
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.90	0.53
1:C:15:TYR:CD1	1:C:33:LYS:NZ	2.77	0.53
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.44	0.53
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.90	0.53
1:C:15:TYR:OH	1:C:47:THR:CB	2.51	0.52
1:C:71:HIS:CG	2:D:300:LYS:NZ	2.76	0.52
2:D:383:THR:O	2:D:384:LEU:C	2.45	0.52
2:D:220:GLU:O	2:D:223:GLU:N	2.42	0.52
1:A:154:VAL:HG13	2:B:179:HIS:CE1	2.44	0.52
1:C:99:ILE:O	1:C:104:ILE:HD11	2.09	0.52
2:D:217:TRP:O	2:D:221:VAL:HG23	2.10	0.52
2:D:326:ASN:OD1	2:D:328:LYS:N	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:388:LYS:O	2:D:392:MET:N	2.40	0.52
2:D:383:THR:C	2:D:385:GLU:N	2.60	0.52
1:C:278:LYS:O	1:C:281:LEU:HB2	2.09	0.52
2:B:395:HIS:HE1	2:B:427:PRO:O	1.92	0.52
1:C:121:HIS:HD2	2:D:185:TYR:CE1	2.28	0.52
2:B:176:PRO:HD3	2:B:179:HIS:NE2	2.25	0.51
1:C:284:PRO:C	1:C:286:PHE:N	2.61	0.51
2:B:296:HIS:O	2:B:300:LYS:HG3	2.10	0.51
2:D:388:LYS:N	2:D:389:PRO:CD	2.73	0.51
2:D:319:PHE:CZ	2:D:330:GLU:HA	2.45	0.51
1:A:137:THR:O	1:A:293:VAL:HG13	2.11	0.51
1:A:72:THR:HG22	1:A:73:GLU:N	2.24	0.51
1:A:0:SER:C	1:A:2:GLU:H	2.14	0.51
2:D:404:HIS:CE1	2:D:406:GLN:HB2	2.46	0.51
2:B:178:TYR:CA	4:B:2009:HOH:O	2.49	0.51
1:C:198:THR:O	1:C:199:ARG:CB	2.57	0.51
1:C:60:HIS:CD2	1:C:61:PRO:CD	2.93	0.51
2:D:357:GLY:O	2:D:358:ALA:C	2.49	0.51
1:C:129:LYS:HB2	1:C:130:PRO:HD2	1.92	0.51
2:B:178:TYR:HB2	4:B:2009:HOH:O	2.11	0.50
2:D:217:TRP:CZ2	2:D:281:ILE:HD12	2.46	0.50
1:A:178:LYS:HE2	1:A:179:TYR:CE1	2.46	0.50
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.92	0.50
1:C:61:PRO:O	1:C:142:LYS:HE2	2.11	0.50
2:D:365:TYR:O	2:D:366:THR:C	2.48	0.50
1:A:33:LYS:HB3	1:A:78:LEU:HB2	1.94	0.50
2:B:207:THR:OG1	2:B:210:MET:HG3	2.12	0.50
1:C:15:TYR:CD1	1:C:33:LYS:HE3	2.43	0.50
1:C:136:ASN:HD21	1:C:140:ALA:HB3	1.75	0.50
1:C:126:ARG:HB3	1:C:163:VAL:HG22	1.94	0.50
2:D:376:LEU:O	2:D:379:LYS:N	2.40	0.50
2:D:354:VAL:O	2:D:355:ILE:C	2.48	0.49
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.47	0.49
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.47	0.49
2:B:190:GLU:HG3	2:B:351:LEU:HD22	1.94	0.49
2:D:184:THR:O	2:D:187:ARG:HB2	2.11	0.49
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.47	0.49
1:C:34:LYS:NZ	1:C:36:ARG:HE	2.10	0.49
1:A:175:LEU:CD1	1:A:233:MET:HE1	2.42	0.49
1:A:64:VAL:HG21	1:A:144:ALA:CB	2.35	0.49
1:C:72:THR:HG22	1:C:73:GLU:H	1.75	0.49
2:D:407:GLN:OE1	2:D:410:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:428:GLU:HG3	2:D:429:THR:HG23	1.93	0.49
1:C:284:PRO:C	1:C:286:PHE:H	2.15	0.49
1:C:195:GLU:O	1:C:199:ARG:N	2.45	0.49
1:A:247:ASP:OD2	1:A:249:SER:OG	2.29	0.49
1:C:15:TYR:HD1	1:C:33:LYS:HZ1	1.56	0.49
2:D:423:LEU:C	2:D:424:LEU:O	2.51	0.49
2:D:423:LEU:O	2:D:424:LEU:C	2.50	0.49
1:C:202:LEU:HD23	1:C:203:PHE:CE1	2.47	0.48
1:C:84:HIS:CD2	1:C:296:LEU:HD13	2.48	0.48
1:A:178:LYS:HE2	1:A:179:TYR:OH	2.14	0.48
1:A:57:GLU:OE2	2:B:307:ALA:HB3	2.13	0.48
1:A:10:ILE:CG2	1:A:10:ILE:O	2.61	0.48
1:A:84:HIS:HB2	4:A:2016:HOH:O	2.13	0.48
2:B:407:GLN:OE1	2:B:410:ARG:HD3	2.13	0.48
2:B:217:TRP:O	2:B:221:VAL:HG23	2.14	0.48
1:C:72:THR:HG22	1:C:74:ASN:H	1.78	0.48
1:A:283:HIS:ND1	1:A:284:PRO:HD2	2.28	0.48
1:C:126:ARG:HD2	1:C:163:VAL:HG21	1.95	0.48
1:C:52:ILE:HD11	1:C:78:LEU:CD2	2.44	0.48
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.95	0.48
1:C:9:LYS:HZ2	1:C:17:VAL:HG22	1.78	0.48
1:C:126:ARG:HB3	1:C:163:VAL:CG2	2.44	0.48
1:C:40:GLU:OE2	2:D:289:LYS:NZ	2.47	0.47
2:D:319:PHE:CG	2:D:330:GLU:HG2	2.49	0.47
1:A:72:THR:HG21	1:A:74:ASN:OD1	2.14	0.47
1:C:266:MET:O	1:C:274:ARG:HD3	2.14	0.47
1:A:262:LEU:HG	1:A:266:MET:HE2	1.97	0.47
1:C:270:ASP:C	1:C:270:ASP:OD1	2.53	0.47
1:A:71:HIS:CE1	2:B:296:HIS:CD2	3.02	0.47
1:C:74:ASN:HB3	4:C:2011:HOH:O	2.14	0.47
2:D:322:GLN:HB3	2:D:324:PRO:O	2.14	0.47
1:A:65:LYS:HA	4:A:2012:HOH:O	2.15	0.47
2:B:235:ALA:O	2:B:239:ILE:HG13	2.14	0.47
1:C:88:LYS:HA	1:C:91:MET:HE2	1.95	0.47
1:A:290:THR:OG1	1:A:292:PRO:HD3	2.15	0.47
2:B:323:GLN:HA	2:B:324:PRO:HA	1.73	0.47
1:C:71:HIS:HB3	2:D:300:LYS:HZ1	1.78	0.47
1:A:39:THR:CG2	1:A:40:GLU:H	2.26	0.47
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.97	0.46
1:C:219:LEU:HB2	1:C:269:TYR:OH	2.15	0.46
2:D:384:LEU:HA	2:D:384:LEU:HD12	1.80	0.46
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:262:LEU:HG	1:A:266:MET:CE	2.45	0.46
2:D:216:ASP:CG	2:D:408:SER:OG	2.53	0.46
2:D:415:ASN:OD1	2:D:416:SER:N	2.47	0.46
2:D:395:HIS:HE1	2:D:427:PRO:O	1.98	0.46
1:A:71:HIS:CD2	2:B:296:HIS:CE1	3.03	0.46
2:D:326:ASN:OD1	2:D:329:VAL:HG23	2.16	0.46
1:A:98:GLY:HA2	1:A:199:ARG:CZ	2.45	0.46
2:D:358:ALA:O	2:D:359:ALA:C	2.53	0.46
2:B:334:MET:HE3	2:B:334:MET:HA	1.98	0.46
2:D:377:ILE:O	2:D:381:GLY:HA2	2.16	0.46
1:A:72:THR:HG21	1:A:74:ASN:ND2	2.30	0.46
1:A:163:VAL:O	1:A:164:VAL:HB	2.16	0.46
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.98	0.46
2:D:230:GLU:OE2	2:D:313:GLN:NE2	2.48	0.46
1:C:157:ARG:HB2	1:C:159:TYR:CE1	2.50	0.46
1:A:39:THR:HG23	2:B:292:LEU:HD23	1.97	0.45
2:B:415:ASN:OD1	2:B:416:SER:N	2.49	0.45
3:E:379:ARG:H	3:E:379:ARG:HG2	1.47	0.45
1:C:283:HIS:CD2	1:C:284:PRO:HD2	2.52	0.45
2:D:385:GLU:OE2	2:D:385:GLU:HA	2.15	0.45
2:B:178:TYR:CB	4:B:2009:HOH:O	2.65	0.45
2:B:280:TYR:HE2	3:E:380:HIS:HE1	1.65	0.45
2:B:196:LYS:HG2	2:B:199:TYR:HB3	1.99	0.45
2:B:312:ASN:ND2	4:B:2042:HOH:O	2.50	0.45
2:B:210:MET:CE	3:E:385:PHE:HB3	2.47	0.45
2:D:377:ILE:O	2:D:381:GLY:N	2.49	0.45
2:D:237:ASN:OD1	2:D:241:ARG:HD3	2.17	0.45
1:C:218:THR:O	1:C:218:THR:HG22	2.16	0.45
1:A:72:THR:CG2	1:A:74:ASN:CG	2.85	0.44
1:C:283:HIS:HA	1:C:284:PRO:HD3	1.86	0.44
2:D:278:PHE:O	2:D:281:ILE:HG13	2.17	0.44
1:C:3:ASN:O	1:C:24:LYS:HG3	2.17	0.44
1:C:202:LEU:HD21	1:C:203:PHE:CZ	2.52	0.44
2:D:383:THR:H	2:D:386:SER:HG	1.65	0.44
1:A:0:SER:C	1:A:2:GLU:N	2.71	0.44
1:C:71:HIS:CB	2:D:300:LYS:HZ3	2.28	0.44
2:B:280:TYR:CE2	3:E:380:HIS:HE1	2.34	0.44
1:C:72:THR:CG2	1:C:73:GLU:H	2.28	0.44
1:A:115:LEU:HD21	1:A:185:ASP:HB3	2.00	0.44
2:B:345:ASP:HA	2:B:346:PRO:HA	1.75	0.44
1:C:289:VAL:HG13	1:C:289:VAL:O	2.18	0.44
1:C:60:HIS:CG	1:C:61:PRO:CD	3.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:197:VAL:HG11	1:A:252:VAL:HG11	1.95	0.44
2:D:326:ASN:CG	2:D:329:VAL:HG23	2.38	0.44
1:C:279:ALA:O	1:C:281:LEU:N	2.51	0.44
2:B:250:ARG:NH1	3:E:386:LYS:OXT	2.51	0.43
2:D:404:HIS:HE1	2:D:406:GLN:OE1	2.02	0.43
1:C:91:MET:O	1:C:92:ASP:C	2.57	0.43
2:D:374:GLU:HA	2:D:377:ILE:HD12	2.00	0.43
1:C:64:VAL:CG2	1:C:144:ALA:CB	2.72	0.43
1:C:15:TYR:CD1	1:C:33:LYS:HE2	2.51	0.43
2:D:310:THR:O	2:D:311:VAL:C	2.55	0.43
1:A:97:THR:HG21	1:A:295:HIS:HE1	1.80	0.43
1:C:202:LEU:CD2	1:C:203:PHE:CE1	3.01	0.43
2:D:395:HIS:HB2	2:D:430:LEU:HD11	1.99	0.43
1:A:278:LYS:NZ	2:B:177:ASP:O	2.33	0.43
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.53	0.43
2:D:215:VAL:O	2:D:219:VAL:HG23	2.18	0.43
2:D:225:TYR:HE1	2:D:281:ILE:HG21	1.84	0.43
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.83	0.43
2:B:210:MET:HE3	3:E:385:PHE:HB3	2.00	0.43
1:A:250:LYS:HA	1:A:250:LYS:HD3	1.83	0.43
1:C:109:PHE:CD2	1:C:113:GLN:NE2	2.87	0.43
2:D:396:GLN:O	2:D:399:LEU:N	2.52	0.43
1:C:9:LYS:HZ3	1:C:17:VAL:CG2	2.32	0.43
2:D:383:THR:O	2:D:386:SER:N	2.51	0.43
2:B:319:PHE:CG	2:B:330:GLU:HG2	2.53	0.43
2:D:216:ASP:OD2	2:D:408:SER:CB	2.67	0.42
1:A:107:TYR:O	1:A:111:LEU:HG	2.19	0.42
1:C:17:VAL:HG11	1:C:19:TYR:OH	2.09	0.42
1:C:35:ILE:HB	1:C:76:LEU:HB3	2.02	0.42
2:D:422:SER:HG	2:D:422:SER:H	1.64	0.42
1:A:72:THR:HG21	1:A:74:ASN:HD21	1.81	0.42
1:C:108:LEU:HD22	1:C:193:PHE:CG	2.54	0.42
1:C:162:GLU:CD	1:C:162:GLU:H	2.22	0.42
1:A:15:TYR:N	1:A:15:TYR:CD1	2.87	0.42
1:A:7:VAL:O	1:A:8:GLU:HB3	2.18	0.42
1:A:294:PRO:C	1:A:296:LEU:H	2.23	0.42
2:D:329:VAL:O	2:D:330:GLU:C	2.58	0.42
1:C:103:LEU:HD11	1:C:107:TYR:CZ	2.54	0.42
1:C:197:VAL:CG1	1:C:252:VAL:CG1	2.95	0.42
1:C:101:LEU:H	1:C:101:LEU:HG	1.66	0.42
2:D:411:GLU:O	2:D:412:LYS:C	2.57	0.42
1:C:115:LEU:CD1	1:C:119:HIS:CE1	3.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:THR:HB	2:B:289:LYS:HZ2	1.81	0.42
1:C:102:PRO:O	1:C:105:LYS:N	2.53	0.42
2:D:394:LEU:HD12	2:D:394:LEU:HA	1.86	0.42
2:D:345:ASP:HA	2:D:346:PRO:HA	1.72	0.42
1:A:72:THR:HG22	1:A:74:ASN:CG	2.40	0.42
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.02	0.42
1:C:129:LYS:HB2	1:C:130:PRO:CD	2.50	0.42
1:A:106:SER:HB2	1:A:290:THR:O	2.20	0.42
1:A:39:THR:O	1:A:40:GLU:HB2	2.20	0.41
1:A:83:LEU:HD21	1:A:142:LYS:HE3	2.02	0.41
1:C:109:PHE:CE2	1:C:113:GLN:NE2	2.88	0.41
1:A:186:ILE:HD11	1:A:277:ALA:HB2	2.02	0.41
1:A:71:HIS:CG	2:B:300:LYS:NZ	2.87	0.41
1:C:284:PRO:O	1:C:285:PHE:C	2.54	0.41
2:D:327:CYS:HG	2:D:419:HIS:CD2	2.34	0.41
1:C:193:PHE:CD1	1:C:266:MET:HE1	2.55	0.41
1:C:270:ASP:OD1	1:C:272:ASN:N	2.53	0.41
2:D:314:PHE:O	2:D:317:GLN:N	2.52	0.41
2:D:364:LEU:HG	2:D:370:GLN:HB2	2.03	0.41
1:A:42:GLU:OE1	2:B:275:VAL:N	2.44	0.41
1:A:134:LEU:O	1:A:141:ILE:HA	2.20	0.41
2:B:219:VAL:HG22	2:B:232:LEU:HD11	2.03	0.41
1:C:167:TRP:CD1	1:C:167:TRP:N	2.87	0.41
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.02	0.41
1:C:60:HIS:HB3	1:C:63:ILE:HD12	2.02	0.41
1:A:72:THR:CG2	1:A:73:GLU:N	2.84	0.41
2:D:210:MET:CE	2:D:250:ARG:CB	2.97	0.41
1:C:284:PRO:O	1:C:286:PHE:N	2.54	0.41
1:C:64:VAL:HG21	1:C:144:ALA:CA	2.50	0.41
1:A:251:VAL:HG12	1:A:252:VAL:HG23	2.02	0.41
2:D:332:LEU:HB3	2:D:363:ALA:HB1	2.02	0.41
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.79	0.41
1:C:279:ALA:O	1:C:280:ALA:C	2.59	0.41
1:A:14:THR:HB	1:A:15:TYR:CD1	2.56	0.41
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.88	0.41
1:C:263:LEU:HD11	1:C:267:LEU:CD1	2.50	0.41
2:B:201:LYS:HB3	2:B:201:LYS:HE3	1.56	0.41
1:C:50:ARG:O	1:C:54:LEU:HG	2.21	0.41
1:A:39:THR:CG2	1:A:40:GLU:N	2.81	0.40
1:A:293:VAL:CG1	1:A:294:PRO:HD2	2.48	0.40
2:D:314:PHE:O	2:D:315:LEU:C	2.60	0.40
2:D:392:MET:O	2:D:395:HIS:HB3	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.04	0.40
2:D:338:GLU:CD	2:D:412:LYS:HZ3	2.24	0.40
1:A:161:HIS:HE1	1:A:173:ILE:O	2.05	0.40
1:A:283:HIS:HA	1:A:284:PRO:HD3	1.92	0.40
2:B:220:GLU:HB3	3:E:379:ARG:HD2	2.03	0.40
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.97	0.40
1:C:15:TYR:OH	1:C:147:GLY:CA	2.68	0.40
1:C:57:GLU:O	1:C:58:LEU:HD23	2.22	0.40
1:A:5:GLN:HE21	1:A:5:GLN:CA	2.33	0.40
1:C:195:GLU:HG3	1:C:200:ARG:C	2.41	0.40
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.93	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	Distance(Å)	Clash(Å)
1:A:199:ARG:NH2	2:B:374:GLU:OE2[4_466]	1.97	0.23

## 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	295/303 (97%)	273 (92%)	19 (6%)	3 (1%)	22	17
1	C	264/303 (87%)	236 (89%)	23 (9%)	5 (2%)	12	5
2	B	256/259 (99%)	252 (98%)	3 (1%)	1 (0%)	43	46
2	D	256/259 (99%)	228 (89%)	22 (9%)	6 (2%)	10	3
3	E	7/11 (64%)	6 (86%)	1 (14%)	0	100	100
All	All	1078/1135 (95%)	995 (92%)	68 (6%)	15 (1%)	16	10

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	VAL

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Mol	Chain	Res	Type
1	C	38	ASP
2	D	420	GLY
2	D	424	LEU
1	A	1	MET
1	A	164	VAL
1	C	145	ASP
2	D	419	HIS
1	A	89	LYS
2	B	176	PRO
1	C	40	GLU
1	C	164	VAL
2	D	176	PRO
2	D	369	GLY
2	D	372	TRP

### 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	261/265 (98%)	239 (92%)	22 (8%)	16	12
1	C	234/265 (88%)	220 (94%)	14 (6%)	27	26
2	B	232/233 (100%)	223 (96%)	9 (4%)	43	51
2	D	232/233 (100%)	221 (95%)	11 (5%)	36	40
3	E	9/11 (82%)	8 (89%)	1 (11%)	9	5
All	All	968/1007 (96%)	911 (94%)	57 (6%)	28	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	9	LYS
1	A	14	THR
1	A	15	TYR
1	A	41	THR
1	A	55	LEU
1	A	59	ASN

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Mol	Chain	Res	Type
1	A	74	ASN
1	A	75	LYS
1	A	78	LEU
1	A	122	ARG
1	A	131	GLN
1	A	148	LEU
1	A	150	ARG
1	A	178	LYS
1	A	206	ASP
1	A	230	VAL
1	A	242	LYS
1	A	247	ASP
1	A	248	PHE
1	A	255	LEU
1	A	268	HIS
2	B	179	HIS
2	B	201	LYS
2	B	232	LEU
2	B	292	LEU
2	B	316	THR
2	B	323	GLN
2	B	334	MET
2	B	384	LEU
2	B	403	GLN
1	C	0	SER
1	C	2	GLU
1	C	9	LYS
1	C	22	ARG
1	C	34	LYS
1	C	36	ARG
1	C	38	ASP
1	C	74	ASN
1	C	75	LYS
1	C	122	ARG
1	C	131	GLN
1	C	150	ARG
1	C	177	CYS
1	C	217	ARG
2	D	179	HIS
2	D	196	LYS
2	D	232	LEU
2	D	245	SER

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Mol	Chain	Res	Type
2	D	292	LEU
2	D	316	THR
2	D	334	MET
2	D	348	LEU
2	D	384	LEU
2	D	386	SER
2	D	398	TYR
3	E	379	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	60	HIS
1	A	62	ASN
1	A	161	HIS
1	A	295	HIS
2	B	179	HIS
2	B	233	HIS
2	B	317	GLN
2	B	395	HIS
2	B	425	ASN
1	C	60	HIS
1	C	84	HIS
1	C	85	GLN
1	C	119	HIS
1	C	121	HIS
2	D	179	HIS
2	D	254	GLN
2	D	317	GLN
2	D	361	HIS
2	D	370	GLN
2	D	395	HIS
2	D	419	HIS
2	D	431	ASN
3	E	380	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	10,10,11	14.51	5 (50%)	12,14,16	3.08	6 (50%)
1	TPO	C	160	1	10,10,11	14.58	5 (50%)	12,14,16	3.30	6 (50%)

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	-	0/9/11/13	0/0/0/0
1	TPO	C	160	1	-	0/9/11/13	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	O-C	45.31	1.42	1.11
1	A	160	TPO	O-C	45.29	1.42	1.11
1	C	160	TPO	P-O1P	5.35	1.69	1.51
1	C	160	TPO	P-O2P	4.20	1.70	1.54
1	A	160	TPO	P-O1P	4.06	1.64	1.51
1	C	160	TPO	P-O3P	3.87	1.68	1.54
1	A	160	TPO	P-O3P	3.60	1.67	1.54
1	A	160	TPO	CA-C	3.29	1.54	1.48
1	A	160	TPO	P-O2P	2.94	1.65	1.54
1	C	160	TPO	CA-C	2.48	1.52	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O2P-P-OG1	-8.41	82.87	107.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O2P-P-OG1	7.20	127.83	107.09
1	C	160	TPO	O2P-P-O1P	3.86	123.06	110.44
1	A	160	TPO	O3P-P-O2P	-3.85	92.63	107.61
1	C	160	TPO	CG2-CB-CA	-3.67	105.67	113.20
1	A	160	TPO	OG1-CB-CA	3.52	113.45	107.55
1	A	160	TPO	OG1-CB-CG2	-3.41	104.42	110.13
1	A	160	TPO	O3P-P-OG1	-3.09	98.20	107.09
1	C	160	TPO	O3P-P-O2P	2.81	118.55	107.61
1	C	160	TPO	OG1-P-O1P	-2.60	99.52	106.79
1	A	160	TPO	CB-CA-N	2.48	113.06	109.60
1	C	160	TPO	P-OG1-CB	2.24	130.06	120.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	297/303 (98%)	0.03	14 (4%) 30 32	20, 29, 74, 105	0
1	C	269/303 (88%)	0.58	33 (12%) 5 6	27, 49, 86, 103	0
2	B	258/259 (99%)	0.43	23 (8%) 10 11	25, 40, 67, 96	0
2	D	258/259 (99%)	0.77	51 (19%) 2 1	26, 43, 73, 103	0
3	E	9/11 (81%)	1.23	1 (11%) 6 7	42, 55, 86, 87	0
All	All	1091/1135 (96%)	0.45	122 (11%) 6 7	20, 41, 79, 105	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	432	LEU	7.8
1	A	297	ARG	7.4
2	D	176	PRO	6.4
1	A	96	LEU	5.9
1	C	253	PRO	5.6
1	A	16	GLY	5.4
1	A	39	THR	5.4
3	E	386	LYS	5.3
1	C	15	TYR	5.1
1	C	297	ARG	5.0
2	D	284	ASP	5.0
2	D	428	GLU	4.8
1	A	15	TYR	4.8
1	C	39	THR	4.8
1	C	295	HIS	4.5
2	D	431	ASN	4.5
2	D	175	VAL	4.4
1	C	296	LEU	4.3
2	D	430	LEU	4.3
2	D	324	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	36	ARG	4.2
1	A	95	ALA	4.1
1	C	189	LEU	4.0
2	D	381	GLY	4.0
2	D	419	HIS	4.0
1	C	175	LEU	4.0
2	D	325	ALA	4.0
1	A	40	GLU	3.9
2	B	175	VAL	3.9
2	D	327	CYS	3.8
1	A	73	GLU	3.8
1	A	277	ALA	3.8
2	D	283	ASP	3.7
2	D	369	GLY	3.6
1	C	273	LYS	3.6
2	D	384	LEU	3.6
1	A	14	THR	3.6
2	D	420	GLY	3.6
1	C	282	ALA	3.5
1	A	97	THR	3.5
1	C	178	LYS	3.5
2	D	372	TRP	3.5
2	D	177	ASP	3.4
2	B	341	LEU	3.4
2	D	323	GLN	3.3
2	B	176	PRO	3.3
1	C	128	LEU	3.3
2	D	378	ARG	3.3
1	C	293	VAL	3.2
1	C	221	THR	3.2
1	C	252	VAL	3.2
1	C	38	ASP	3.2
2	B	256	VAL	3.1
1	C	287	GLN	3.0
1	C	288	ASP	3.0
2	D	377	ILE	3.0
2	D	423	LEU	2.9
2	D	399	LEU	2.9
2	B	355	ILE	2.9
2	D	424	LEU	2.9
2	D	328	LYS	2.9
2	D	383	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	280	TYR	2.9
2	D	365	TYR	2.8
2	D	390	CYS	2.8
2	B	235	ALA	2.8
1	C	162	GLU	2.8
2	D	385	GLU	2.8
2	D	392	MET	2.8
1	C	256	ASP	2.8
1	C	251	VAL	2.7
2	B	198	GLY	2.7
2	B	236	VAL	2.6
2	B	432	LEU	2.6
1	C	179	TYR	2.6
2	D	418	TYR	2.6
2	D	367	VAL	2.6
1	C	176	GLY	2.6
1	A	296	LEU	2.5
1	C	133	LEU	2.5
2	D	391	LEU	2.5
2	D	395	HIS	2.5
1	C	177	CYS	2.5
2	B	431	ASN	2.5
2	D	280	TYR	2.5
2	D	360	PHE	2.4
2	B	218	LEU	2.4
1	C	257	GLU	2.4
2	B	239	ILE	2.3
2	D	427	PRO	2.3
1	C	97	THR	2.3
2	D	426	PRO	2.3
2	D	388	LYS	2.3
2	D	361	HIS	2.3
2	D	429	THR	2.3
1	C	258	ASP	2.3
1	C	14	THR	2.3
2	B	232	LEU	2.3
2	B	234	LEU	2.3
2	B	315	LEU	2.2
1	C	16	GLY	2.2
2	D	350	TYR	2.2
2	D	382	TYR	2.2
2	B	323	GLN	2.2

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
2	D	417	LYS	2.1
2	D	179	HIS	2.1
2	D	326	ASN	2.1
1	A	71	HIS	2.1
2	B	337	GLY	2.1
2	B	179	HIS	2.1
2	B	325	ALA	2.1
2	D	375	SER	2.1
2	D	374	GLU	2.1
1	C	102	PRO	2.1
2	B	428	GLU	2.1
1	C	188	SER	2.1
2	B	403	GLN	2.0
2	D	320	LEU	2.0
2	D	425	ASN	2.0
1	C	74	ASN	2.0
2	B	257	GLY	2.0
2	D	363	ALA	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	A	160	11/12	0.10	-0.36	21,30,35,38	0
1	TPO	C	160	11/12	0.09	-1.22	39,43,44,47	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.