



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 08:02 AM GMT

PDB ID : 1H24  
Title : CDK2/CYCLIN A IN COMPLEX WITH A 9 RESIDUE RECRUITMENT PEPTIDE FROM E2F  
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 : 2.50 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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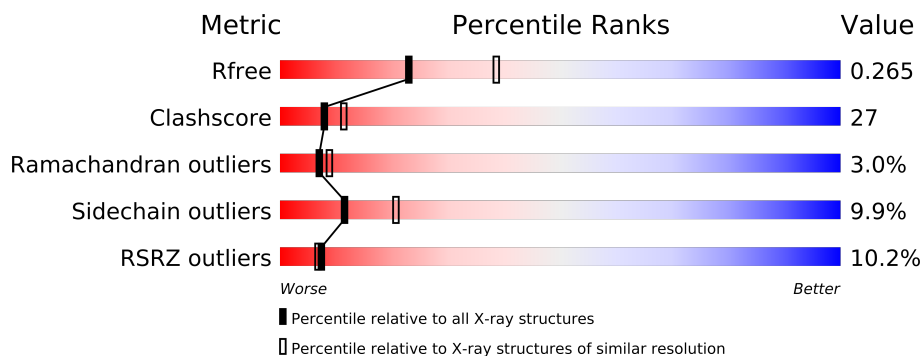
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	9	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9201 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	294	Total	C	N	O	P	S	0	0	0
			2363	1533	399	422	1	8			
1	C	294	Total	C	N	O	P	S	0	0	0
			2363	1533	399	422	1	8			

- 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
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

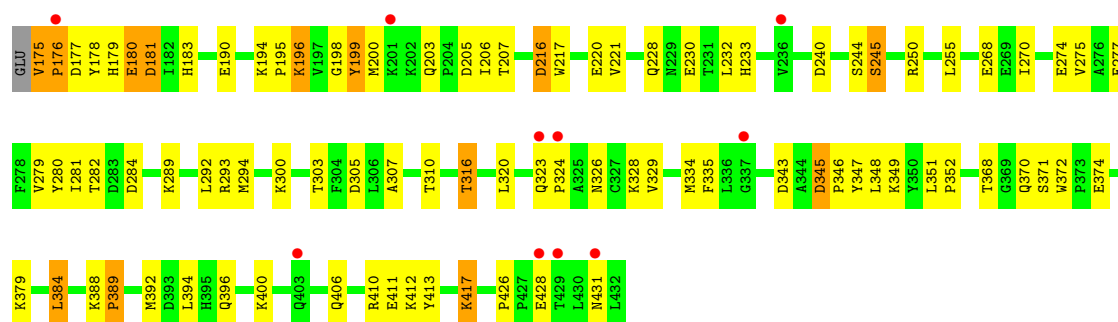
- Molecule 3 is a protein called TRANSCRIPTION FACTOR E2F1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	0	0	0
			78	49	16	13			

- Molecule 4 is water.

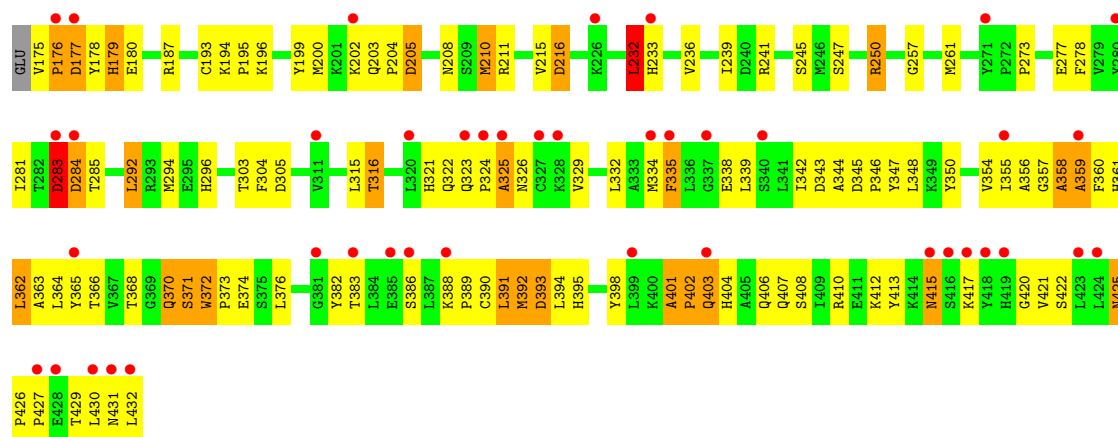
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	75	Total	O	0	0
			75	75		
4	C	40	Total	O	0	0
			40	40		
4	D	40	Total	O	0	0
			40	40		
4	E	1	Total	O	0	0
			1	1		





### • Molecule 2: CYCLIN A2

Chain D:



### • Molecule 3: TRANSCRIPTION FACTOR E2F1

Chain E:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.55Å 133.55Å 147.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.80 – 2.50 28.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.7 (28.80-2.50) 94.7 (28.88-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.209 , 0.270 0.207 , 0.265	Depositor DCC
$R_{free}$ test set	2470 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 36.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 48426 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9201	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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

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	0.92	1/2411 (0.0%)	1.08	9/3270 (0.3%)
1	C	0.75	1/2411 (0.0%)	0.98	12/3270 (0.4%)
2	B	0.90	0/2133	1.02	9/2897 (0.3%)
2	D	0.69	0/2133	0.89	6/2897 (0.2%)
3	E	0.69	0/78	0.98	0/102
All	All	0.82	2/9166 (0.0%)	1.00	36/12436 (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	2
1	C	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	GLU	CD-OE2	10.05	1.36	1.25
1	C	129	LYS	CE-NZ	6.79	1.66	1.49

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ASP	CB-CG-OD2	9.99	127.29	118.30
2	B	305	ASP	CB-CG-OD2	9.36	126.72	118.30
2	B	205	ASP	CB-CG-OD2	7.85	125.37	118.30
1	A	127	ASP	CB-CG-OD2	7.78	125.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	181	ASP	CB-CG-OD2	7.40	124.96	118.30
2	B	216	ASP	CB-CG-OD2	7.18	124.76	118.30
2	B	345	ASP	CB-CG-OD2	6.86	124.47	118.30
2	D	305	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	256	ASP	CB-CG-OD2	6.65	124.29	118.30
2	D	216	ASP	CB-CG-OD2	6.64	124.28	118.30
1	C	206	ASP	CB-CG-OD2	6.42	124.07	118.30
2	D	283	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	235	ASP	CB-CG-OD2	6.29	123.97	118.30
1	C	185	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	288	ASP	CB-CG-OD2	6.24	123.92	118.30
2	D	205	ASP	CB-CG-OD2	6.17	123.85	118.30
1	C	50	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	59	ASN	CB-CA-C	5.92	122.25	110.40
1	C	256	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	98	GLY	N-CA-C	-5.78	98.66	113.10
1	A	223	ASP	CB-CG-OD2	5.77	123.50	118.30
1	C	126	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	C	68	ASP	CB-CG-OD2	5.72	123.44	118.30
2	B	410	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	C	38	ASP	CB-CG-OD2	5.61	123.35	118.30
2	B	343	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	247	ASP	CB-CG-OD2	5.59	123.33	118.30
2	B	240	ASP	CB-CG-OD2	5.54	123.28	118.30
2	D	232	LEU	CB-CG-CD1	-5.50	101.64	111.00
1	A	210	ASP	CB-CG-OD2	5.46	123.22	118.30
1	C	210	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	235	ASP	CB-CG-OD2	5.33	123.10	118.30
2	B	410	ARG	NE-CZ-NH1	-5.24	117.68	120.30
2	D	177	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	20	LYS	N-CA-C	-5.17	97.03	111.00
1	C	127	ASP	CB-CG-OD2	5.06	122.86	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	TYR	Mainchain
1	A	160	TPO	Mainchain
1	C	159	TYR	Mainchain
1	C	160	TPO	Mainchain



## 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	2363	0	2403	135	1
1	C	2363	0	2404	154	0
2	B	2083	0	2107	82	1
2	D	2083	0	2106	135	0
3	E	78	0	87	8	0
4	A	75	0	0	19	0
4	B	75	0	0	16	0
4	C	40	0	0	10	0
4	D	40	0	0	7	0
4	E	1	0	0	0	0
All	All	9201	0	9107	488	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 27.

All (488) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:88:LYS:CD	1:A:131:GLN:HE21	1.43	1.29
2:B:175:VAL:N	2:B:179:HIS:HE1	1.30	1.27
4:A:2023:HOH:O	2:B:300:LYS:HB2	1.27	1.27
2:B:245:SER:HB3	4:B:2021:HOH:O	1.29	1.25
1:C:10:ILE:HD11	4:C:2014:HOH:O	1.33	1.23
2:B:175:VAL:N	2:B:179:HIS:CE1	2.09	1.18
1:A:88:LYS:HD2	1:A:131:GLN:NE2	1.61	1.15
1:C:88:LYS:CB	1:C:131:GLN:HE21	1.59	1.14
1:C:88:LYS:HB2	1:C:131:GLN:HE21	0.99	1.14
1:C:72:THR:HG22	1:C:75:LYS:H	1.14	1.13
1:A:71:HIS:HB2	4:A:2022:HOH:O	1.53	1.08
1:A:88:LYS:HD2	1:A:131:GLN:HE21	1.14	1.07
1:C:154:VAL:O	2:D:316:THR:HG22	1.54	1.07
1:A:2:GLU:HB2	1:C:73:GLU:OE1	1.55	1.07
1:A:177:CYS:HB3	4:A:2046:HOH:O	1.56	1.06
2:D:326:ASN:OD1	2:D:329:VAL:N	1.90	1.05
1:C:126:ARG:NH1	1:C:180:TYR:OH	1.89	1.04

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:205:ASP:OD1	2:D:250:ARG:NH2	1.89	1.04
1:C:88:LYS:HB2	1:C:131:GLN:NE2	1.72	1.04
1:A:88:LYS:HD3	1:A:131:GLN:HE21	1.21	1.01
1:C:96:LEU:N	1:C:96:LEU:HD23	1.76	1.01
1:C:227:TRP:O	1:C:230:VAL:HG23	1.60	1.00
1:C:60:HIS:HD2	1:C:62:ASN:H	1.09	0.99
2:D:329:VAL:HG21	2:D:364:LEU:HD12	1.42	0.99
2:D:358:ALA:O	2:D:360:PHE:N	1.96	0.98
1:A:154:VAL:O	2:B:316:THR:HG22	1.60	0.98
2:D:404:HIS:O	2:D:407:GLN:NE2	1.95	0.98
2:B:178:TYR:HB2	4:B:2009:HOH:O	1.63	0.98
1:A:88:LYS:CD	1:A:131:GLN:NE2	2.18	0.98
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.45	0.96
2:D:415:ASN:OD1	2:D:417:LYS:N	1.99	0.96
1:C:88:LYS:HG3	1:C:131:GLN:NE2	1.84	0.93
1:C:237:LYS:O	4:C:2036:HOH:O	1.87	0.93
2:D:233:HIS:HD2	4:D:2031:HOH:O	1.53	0.92
1:C:105:LYS:HG3	1:C:285:PHE:CE2	2.04	0.92
1:C:60:HIS:CD2	1:C:62:ASN:H	1.90	0.89
1:C:121:HIS:O	1:C:122:ARG:HG3	1.74	0.88
2:D:250:ARG:CD	4:D:2015:HOH:O	2.20	0.87
2:D:250:ARG:HD2	4:D:2015:HOH:O	1.73	0.87
1:A:71:HIS:ND1	4:A:2022:HOH:O	2.08	0.85
1:C:15:TYR:CD1	1:C:35:ILE:HG12	2.11	0.85
1:A:37:LEU:O	1:A:38:ASP:HB2	1.75	0.84
2:D:329:VAL:CG2	2:D:364:LEU:HA	2.08	0.84
1:C:88:LYS:CG	1:C:131:GLN:NE2	2.42	0.83
2:D:360:PHE:HE2	2:D:376:LEU:CD1	1.92	0.82
1:C:198:THR:O	1:C:199:ARG:O	1.98	0.81
1:C:154:VAL:O	2:D:316:THR:CG2	2.28	0.81
2:B:250:ARG:HH11	3:E:95:GLU:HA	1.45	0.81
1:A:98:GLY:HA2	1:A:199:ARG:NE	1.94	0.81
1:C:283:HIS:ND1	1:C:284:PRO:HD2	1.95	0.80
1:C:88:LYS:CB	1:C:131:GLN:NE2	2.39	0.80
2:B:274:GLU:HG2	2:B:277:GLU:OE2	1.82	0.79
1:A:60:HIS:CD2	1:A:62:ASN:H	2.00	0.79
1:C:88:LYS:CG	1:C:131:GLN:HE21	1.95	0.79
2:D:360:PHE:HE2	2:D:376:LEU:HD11	1.47	0.78
2:B:195:PRO:HD2	4:B:2012:HOH:O	1.83	0.78
2:D:329:VAL:HG21	2:D:364:LEU:HA	1.66	0.77
1:C:121:HIS:C	1:C:122:ARG:HG3	2.05	0.77
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.65	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:230:GLU:HA	2:B:230:GLU:OE1	1.84	0.76
1:C:105:LYS:HD3	1:C:285:PHE:O	1.85	0.76
2:D:393:ASP:HA	4:D:2035:HOH:O	1.86	0.76
1:C:71:HIS:CD2	2:D:296:HIS:NE2	2.54	0.76
1:C:71:HIS:HD2	2:D:296:HIS:NE2	1.84	0.75
2:B:417:LYS:HZ2	2:B:417:LYS:HB2	1.51	0.75
1:A:97:THR:OG1	1:A:98:GLY:O	2.04	0.75
1:C:72:THR:HG22	1:C:75:LYS:N	1.97	0.75
2:D:323:GLN:N	2:D:324:PRO:HD3	2.02	0.75
2:D:350:TYR:CD1	2:D:390:CYS:HB2	2.22	0.75
2:D:360:PHE:CE2	2:D:376:LEU:CD1	2.70	0.75
1:A:154:VAL:O	2:B:316:THR:CG2	2.35	0.74
1:C:256:ASP:O	1:C:260:ARG:HG3	1.86	0.74
1:A:39:THR:HG22	1:A:40:GLU:N	2.01	0.74
1:A:290:THR:O	1:A:292:PRO:HD3	1.87	0.74
1:C:240:PHE:HB2	4:C:2036:HOH:O	1.87	0.73
2:D:415:ASN:CG	2:D:417:LYS:H	1.89	0.73
2:D:346:PRO:HD2	2:D:347:TYR:CD2	2.23	0.73
1:A:10:ILE:HD11	1:A:82:PHE:HE1	1.53	0.73
2:D:210:MET:CE	2:D:250:ARG:HB2	2.19	0.72
1:A:96:LEU:O	1:A:97:THR:C	2.27	0.72
2:D:360:PHE:CE2	2:D:376:LEU:HD11	2.25	0.72
1:A:97:THR:OG1	1:A:98:GLY:N	2.22	0.72
2:B:175:VAL:HG13	2:B:175:VAL:O	1.90	0.72
2:B:417:LYS:NZ	2:B:417:LYS:CB	2.53	0.72
1:A:88:LYS:HD3	1:A:131:GLN:NE2	1.96	0.72
1:A:39:THR:HG22	1:A:40:GLU:H	1.55	0.72
2:B:323:GLN:HA	2:B:323:GLN:OE1	1.88	0.72
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.25	0.71
2:D:200:MET:HG2	2:D:208:ASN:OD1	1.90	0.71
2:D:323:GLN:N	2:D:324:PRO:CD	2.53	0.71
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.71	0.71
2:D:401:ALA:HB3	2:D:402:PRO:CD	2.19	0.71
1:C:61:PRO:O	1:C:142:LYS:HE2	1.90	0.71
1:A:60:HIS:HD2	1:A:62:ASN:H	1.35	0.71
1:A:290:THR:C	1:A:292:PRO:HD3	2.11	0.71
1:A:129:LYS:NZ	1:A:165:THR:OG1	2.23	0.71
1:C:278:LYS:NZ	2:D:177:ASP:O	2.21	0.70
2:D:415:ASN:OD1	2:D:417:LYS:CB	2.40	0.70
1:C:251:VAL:HG12	1:C:252:VAL:HG23	1.74	0.70
1:A:161:HIS:O	1:A:163:VAL:N	2.24	0.70
1:C:62:ASN:ND2	1:C:141:ILE:O	2.21	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:222:PRO:HG3	1:C:269:TYR:CZ	2.28	0.69
2:D:357:GLY:O	2:D:358:ALA:O	2.09	0.69
1:A:38:ASP:O	1:A:39:THR:HB	1.90	0.69
2:D:372:TRP:CZ3	2:D:376:LEU:HD13	2.28	0.69
2:B:195:PRO:HB2	4:B:2012:HOH:O	1.91	0.69
1:C:198:THR:C	1:C:199:ARG:O	2.30	0.69
1:C:95:ALA:O	1:C:199:ARG:NH1	2.26	0.69
3:E:87:PRO:O	3:E:90:ARG:HD3	1.94	0.68
1:A:97:THR:N	4:A:2027:HOH:O	2.25	0.68
2:D:199:TYR:CE1	2:D:200:MET:HE2	2.29	0.68
2:D:210:MET:HE2	2:D:250:ARG:HB2	1.76	0.68
1:A:217:ARG:HG2	1:A:243:TRP:CD2	2.29	0.68
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.75	0.67
2:D:368:THR:OG1	2:D:370:GLN:HG3	1.94	0.67
1:C:247:ASP:OD2	1:C:249:SER:OG	2.12	0.67
1:C:58:LEU:HD23	1:C:58:LEU:H	1.60	0.67
2:B:417:LYS:NZ	2:B:417:LYS:HB2	2.09	0.67
1:A:290:THR:O	1:A:292:PRO:CD	2.43	0.66
2:B:323:GLN:OE1	2:B:324:PRO:HA	1.93	0.66
2:D:329:VAL:HG22	2:D:364:LEU:HA	1.76	0.66
1:C:35:ILE:O	1:C:35:ILE:HG22	1.96	0.66
2:D:350:TYR:CE1	2:D:390:CYS:HB2	2.31	0.66
1:A:34:LYS:HD3	1:A:75:LYS:HD2	1.77	0.66
1:C:105:LYS:HE2	1:C:285:PHE:CE1	2.31	0.66
1:C:3:ASN:HB2	4:C:2004:HOH:O	1.96	0.66
1:A:163:VAL:CG1	1:A:164:VAL:HG23	2.26	0.66
2:D:199:TYR:CE1	2:D:200:MET:CE	2.79	0.65
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.79	0.65
1:A:121:HIS:O	1:A:122:ARG:HG3	1.97	0.65
1:C:137:THR:O	4:C:2019:HOH:O	2.14	0.65
1:C:161:HIS:O	1:C:163:VAL:N	2.30	0.65
1:A:51:GLU:OE2	4:A:2016:HOH:O	2.14	0.64
2:D:338:GLU:OE1	2:D:412:LYS:NZ	2.31	0.64
1:C:195:GLU:O	1:C:199:ARG:N	2.31	0.64
1:C:72:THR:HG23	1:C:73:GLU:N	2.12	0.64
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.33	0.64
2:D:199:TYR:HE1	2:D:200:MET:HE1	1.63	0.63
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.81	0.63
2:B:176:PRO:HB2	4:B:2008:HOH:O	1.99	0.63
1:C:227:TRP:O	1:C:230:VAL:CG2	2.42	0.63
1:A:101:LEU:N	1:A:102:PRO:CD	2.60	0.63
2:D:216:ASP:HB2	2:D:406:GLN:HG2	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:252:VAL:HG12	1:C:255:LEU:HB2	1.80	0.63
2:B:346:PRO:O	2:B:349:LYS:HG2	1.98	0.63
2:D:354:VAL:O	2:D:357:GLY:N	2.32	0.62
1:A:163:VAL:HG12	1:A:164:VAL:HG23	1.79	0.62
1:A:39:THR:CG2	1:A:40:GLU:H	2.11	0.62
1:A:39:THR:HG21	2:B:289:LYS:CD	2.28	0.62
1:C:72:THR:CG2	1:C:75:LYS:H	2.02	0.62
1:A:156:VAL:HB	1:A:159:TYR:CE2	2.34	0.62
2:D:199:TYR:HE1	2:D:200:MET:CE	2.13	0.62
2:D:338:GLU:CD	2:D:412:LYS:HZ3	2.03	0.62
1:C:155:PRO:C	4:C:2021:HOH:O	2.38	0.62
2:D:361:HIS:O	2:D:363:ALA:N	2.33	0.61
2:B:176:PRO:HA	2:B:179:HIS:CG	2.35	0.61
2:B:198:GLY:O	2:B:200:MET:N	2.33	0.61
2:D:284:ASP:N	2:D:284:ASP:OD1	2.33	0.61
1:C:105:LYS:HG3	1:C:285:PHE:CZ	2.35	0.61
1:A:60:HIS:HE1	4:A:2032:HOH:O	1.82	0.61
2:D:362:LEU:HD21	2:D:398:TYR:HD2	1.66	0.61
1:C:293:VAL:C	4:C:2039:HOH:O	2.39	0.61
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.83	0.61
1:C:156:VAL:HG23	1:C:156:VAL:O	2.00	0.61
2:D:401:ALA:CB	2:D:402:PRO:HD3	2.25	0.61
2:D:346:PRO:HD2	2:D:347:TYR:CE2	2.36	0.61
2:D:388:LYS:O	2:D:392:MET:N	2.31	0.61
2:D:329:VAL:HG11	2:D:364:LEU:HD13	1.83	0.61
2:D:329:VAL:HG21	2:D:364:LEU:CD1	2.24	0.60
1:A:86:ASP:C	1:A:86:ASP:OD1	2.39	0.60
2:B:255:LEU:HG	2:B:294:MET:HG2	1.83	0.60
1:C:72:THR:HG23	1:C:74:ASN:H	1.67	0.60
2:B:178:TYR:CA	4:B:2009:HOH:O	2.49	0.60
2:D:211:ARG:O	2:D:215:VAL:HG23	2.02	0.60
2:D:211:ARG:HH11	2:D:211:ARG:HG2	1.67	0.60
1:C:95:ALA:C	1:C:96:LEU:HD23	2.22	0.59
2:D:415:ASN:OD1	2:D:417:LYS:CA	2.50	0.59
2:B:183:HIS:HE1	4:B:2045:HOH:O	1.84	0.59
1:C:58:LEU:HD23	1:C:58:LEU:N	2.16	0.59
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.85	0.59
1:A:39:THR:CG2	1:A:40:GLU:N	2.65	0.59
1:C:163:VAL:HG13	1:C:164:VAL:HG23	1.84	0.59
1:C:283:HIS:CE1	1:C:284:PRO:HD2	2.38	0.59
1:A:231:THR:HG22	1:A:236:TYR:CZ	2.38	0.58
2:B:175:VAL:O	2:B:177:ASP:N	2.36	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.39	0.58
2:D:273:PRO:HB2	2:D:278:PHE:CE2	2.39	0.58
1:C:0:SER:HA	4:C:2001:HOH:O	2.04	0.58
1:C:15:TYR:CE1	1:C:35:ILE:HG12	2.39	0.58
1:C:2:GLU:OE1	1:C:3:ASN:OD1	2.22	0.58
1:A:57:GLU:OE2	2:B:307:ALA:HB3	2.04	0.57
2:D:332:LEU:HD12	2:D:335:PHE:HE2	1.69	0.57
2:D:211:ARG:NH1	2:D:211:ARG:HG2	2.18	0.57
1:A:121:HIS:C	1:A:122:ARG:HG3	2.25	0.57
1:C:60:HIS:HD2	1:C:62:ASN:N	1.91	0.57
2:D:176:PRO:HA	2:D:179:HIS:CG	2.39	0.57
1:A:217:ARG:HG2	1:A:243:TRP:CE2	2.39	0.57
1:C:205:GLY:HA2	1:C:210:ASP:OD2	2.05	0.57
2:D:281:ILE:C	2:D:283:ASP:H	2.07	0.57
1:C:268:HIS:CD2	1:C:273:LYS:HB2	2.40	0.56
1:A:16:GLY:HA3	4:A:2010:HOH:O	2.05	0.56
2:B:178:TYR:CB	4:B:2009:HOH:O	2.34	0.56
1:A:71:HIS:CB	4:A:2022:HOH:O	2.27	0.56
2:B:195:PRO:CB	4:B:2012:HOH:O	2.51	0.56
1:A:289:VAL:HG22	1:A:290:THR:N	2.21	0.56
2:B:280:TYR:HD1	4:B:2035:HOH:O	1.88	0.56
2:D:358:ALA:HA	2:D:391:LEU:HD22	1.87	0.56
2:D:216:ASP:OD1	2:D:408:SER:OG	2.24	0.55
2:B:180:GLU:OE1	2:B:379:LYS:NZ	2.37	0.55
1:A:64:VAL:HG13	1:A:64:VAL:O	2.06	0.55
1:A:170:ALA:HB1	1:A:171:PRO:HD2	1.87	0.55
2:D:401:ALA:O	2:D:403:GLN:N	2.39	0.55
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.36	0.55
1:C:0:SER:CA	4:C:2001:HOH:O	2.55	0.55
1:C:60:HIS:CG	1:C:61:PRO:CD	2.90	0.54
1:C:84:HIS:CE1	1:C:136:ASN:C	2.80	0.54
2:B:178:TYR:N	4:B:2009:HOH:O	2.33	0.54
1:A:37:LEU:O	1:A:38:ASP:CB	2.49	0.54
3:E:88:VAL:O	3:E:90:ARG:N	2.41	0.54
2:D:362:LEU:HD21	2:D:398:TYR:CD2	2.42	0.54
1:A:71:HIS:CG	4:A:2022:HOH:O	2.43	0.54
1:C:174:LEU:HD11	1:C:211:GLN:HG2	1.88	0.54
1:A:96:LEU:O	1:A:98:GLY:N	2.41	0.54
2:D:417:LYS:HB3	2:D:417:LYS:NZ	2.23	0.54
1:A:39:THR:HG22	1:A:40:GLU:HG3	1.89	0.54
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.37	0.54
2:D:193:CYS:O	2:D:241:ARG:HD2	2.07	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:338:GLU:CD	2:D:412:LYS:NZ	2.61	0.53
1:C:83:LEU:HD23	1:C:136:ASN:HB3	1.90	0.53
2:D:358:ALA:O	2:D:359:ALA:C	2.45	0.53
1:A:97:THR:CA	4:A:2027:HOH:O	2.56	0.53
2:D:415:ASN:ND2	4:D:2037:HOH:O	2.37	0.53
2:B:289:LYS:HE3	2:B:293:ARG:HH21	1.72	0.53
1:A:106:SER:HB2	1:A:290:THR:O	2.09	0.53
2:B:176:PRO:HG3	2:B:179:HIS:NE2	2.24	0.53
1:A:174:LEU:CD2	1:A:208:GLU:HG2	2.38	0.53
2:D:210:MET:HE1	2:D:250:ARG:HB2	1.89	0.53
2:D:323:GLN:H	2:D:324:PRO:HD3	1.74	0.53
1:C:157:ARG:HG3	1:C:158:THR:N	2.23	0.53
2:D:354:VAL:O	2:D:355:ILE:C	2.48	0.52
2:D:335:PHE:HB3	2:D:413:TYR:CD2	2.44	0.52
1:A:103:LEU:HD13	1:A:292:PRO:HB2	1.91	0.52
2:D:232:LEU:O	2:D:236:VAL:HG23	2.09	0.52
2:D:361:HIS:O	2:D:362:LEU:C	2.47	0.52
2:D:250:ARG:HD3	4:D:2015:HOH:O	1.95	0.52
1:A:39:THR:HG21	2:B:289:LYS:HD2	1.90	0.52
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.44	0.52
2:B:195:PRO:CD	4:B:2012:HOH:O	2.49	0.52
1:A:85:GLN:OE1	1:A:89:LYS:HG2	2.09	0.52
2:B:175:VAL:CG1	2:B:175:VAL:O	2.55	0.52
1:C:195:GLU:O	1:C:199:ARG:CA	2.58	0.52
2:B:417:LYS:HB3	2:B:417:LYS:HZ3	1.75	0.52
1:C:108:LEU:HD22	1:C:193:PHE:CD1	2.44	0.52
2:D:332:LEU:HD12	2:D:335:PHE:CE2	2.45	0.52
1:A:207:SER:H	1:A:210:ASP:HB3	1.74	0.52
1:C:2:GLU:HG2	1:C:2:GLU:O	2.09	0.51
2:B:183:HIS:CE1	4:B:2045:HOH:O	2.59	0.51
1:C:72:THR:CG2	1:C:74:ASN:H	2.23	0.51
1:C:174:LEU:HD11	1:C:211:GLN:CG	2.40	0.51
1:A:34:LYS:HG3	1:A:77:TYR:CE1	2.46	0.51
1:C:252:VAL:CG1	1:C:255:LEU:HB2	2.41	0.51
1:C:54:LEU:O	1:C:58:LEU:HG	2.10	0.51
4:A:2070:HOH:O	2:B:177:ASP:HB3	2.11	0.51
1:A:230:VAL:O	1:A:233:MET:HG3	2.11	0.51
3:E:94:LEU:O	3:E:95:GLU:C	2.49	0.51
1:C:39:THR:O	1:C:40:GLU:HB2	2.10	0.51
1:C:231:THR:HA	1:C:236:TYR:CD1	2.46	0.51
3:E:93:ASP:C	3:E:94:LEU:HD23	2.31	0.50
1:C:91:MET:CE	1:C:130:PRO:HB3	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:135:ILE:HG22	1:C:141:ILE:HG13	1.94	0.50
1:A:98:GLY:CA	1:A:199:ARG:NE	2.72	0.50
2:B:347:TYR:OH	2:B:394:LEU:HA	2.11	0.50
1:C:156:VAL:O	1:C:156:VAL:CG2	2.59	0.50
2:D:176:PRO:HA	2:D:179:HIS:ND1	2.26	0.50
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.94	0.50
2:D:347:TYR:OH	2:D:394:LEU:HA	2.11	0.50
1:A:96:LEU:C	4:A:2027:HOH:O	2.49	0.50
1:A:51:GLU:O	1:A:55:LEU:HB2	2.12	0.50
1:A:129:LYS:HB2	1:A:130:PRO:CD	2.42	0.49
2:B:176:PRO:HG3	2:B:179:HIS:CD2	2.46	0.49
2:D:338:GLU:OE2	2:D:412:LYS:NZ	2.35	0.49
2:B:196:LYS:HG2	2:B:244:SER:HB3	1.93	0.49
2:D:420:GLY:O	2:D:422:SER:N	2.45	0.49
1:A:94:SER:O	1:A:98:GLY:N	2.41	0.49
1:C:241:PRO:HG2	1:C:243:TRP:CH2	2.47	0.49
2:B:351:LEU:HB3	2:B:352:PRO:HD2	1.93	0.49
1:C:51:GLU:O	1:C:55:LEU:HB2	2.12	0.49
1:A:95:ALA:O	1:A:199:ARG:NH1	2.45	0.49
1:A:110:GLN:OE1	1:A:140:ALA:HA	2.12	0.49
1:A:106:SER:HB2	1:A:292:PRO:HD2	1.93	0.49
1:C:164:VAL:HG12	1:C:165:THR:O	2.13	0.49
1:A:124:LEU:CD2	1:A:182:THR:HA	2.42	0.49
1:A:223:ASP:OD1	1:A:223:ASP:C	2.51	0.49
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.48	0.49
1:C:222:PRO:HG3	1:C:269:TYR:CE1	2.46	0.49
1:C:239:SER:O	1:C:240:PHE:C	2.50	0.49
1:C:16:GLY:HA3	1:C:34:LYS:O	2.12	0.49
1:A:256:ASP:HB3	4:A:2065:HOH:O	2.12	0.49
1:C:72:THR:CG2	1:C:73:GLU:N	2.76	0.49
1:A:119:HIS:HD2	4:A:2071:HOH:O	1.96	0.49
1:C:256:ASP:OD2	1:C:258:ASP:HB2	2.12	0.48
1:C:266:MET:O	1:C:274:ARG:HD3	2.12	0.48
1:C:85:GLN:OE1	1:C:89:LYS:HG2	2.13	0.48
1:A:231:THR:HA	1:A:236:TYR:CD1	2.48	0.48
3:E:91:ARG:O	3:E:91:ARG:HG3	2.13	0.48
1:C:163:VAL:O	1:C:164:VAL:HB	2.14	0.48
1:C:155:PRO:O	1:C:155:PRO:HG2	2.13	0.48
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.96	0.48
1:C:110:GLN:OE1	1:C:140:ALA:HA	2.14	0.48
1:C:60:HIS:CD2	1:C:61:PRO:CD	2.95	0.48
1:A:227:TRP:CE3	1:A:269:TYR:HB3	2.49	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:98:GLY:HA2	1:A:199:ARG:CD	2.43	0.48
1:C:231:THR:HG22	1:C:236:TYR:CZ	2.49	0.48
1:C:163:VAL:CG1	1:C:164:VAL:HG23	2.43	0.47
1:A:39:THR:C	1:A:41:THR:N	2.67	0.47
1:C:187:TRP:CZ2	1:C:215:ILE:HD13	2.50	0.47
1:A:25:LEU:HB3	2:D:294:MET:CE	2.44	0.47
2:B:345:ASP:HA	2:B:346:PRO:HA	1.64	0.47
1:C:39:THR:O	1:C:41:THR:N	2.47	0.47
1:A:56:LYS:NZ	2:B:303:THR:O	2.40	0.47
1:A:289:VAL:HG22	1:A:290:THR:H	1.79	0.47
1:A:64:VAL:CG1	1:A:64:VAL:O	2.62	0.47
1:C:150:ARG:HD3	1:C:151:ALA:O	2.14	0.47
1:A:157:ARG:NH1	2:B:268:GLU:OE2	2.37	0.47
2:D:239:ILE:HD11	2:D:257:GLY:HA2	1.97	0.47
2:B:426:PRO:CD	4:B:2004:HOH:O	2.62	0.47
1:A:249:SER:HA	1:A:260:ARG:HD3	1.97	0.47
1:A:160:TPO:O1P	2:B:270:ILE:HA	2.15	0.47
1:C:212:LEU:HD23	1:C:212:LEU:HA	1.50	0.47
1:C:111:LEU:HD21	1:C:141:ILE:HD13	1.97	0.47
2:D:175:VAL:CG2	2:D:176:PRO:HD2	2.45	0.47
2:D:332:LEU:CD2	2:D:363:ALA:HA	2.44	0.46
1:A:155:PRO:HG3	2:B:320:LEU:HD21	1.97	0.46
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.71	0.46
2:B:250:ARG:HH11	3:E:95:GLU:CA	2.23	0.46
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.41	0.46
2:B:396:GLN:HE21	2:B:400:LYS:HE3	1.81	0.46
1:C:133:LEU:C	1:C:134:LEU:HD23	2.36	0.46
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.45	0.46
2:B:323:GLN:HA	2:B:324:PRO:HA	1.56	0.46
1:C:57:GLU:HB2	1:C:58:LEU:H	1.36	0.46
1:C:213:PHE:O	1:C:217:ARG:HG2	2.16	0.46
2:D:315:LEU:HD23	2:D:356:ALA:HB1	1.97	0.46
1:A:39:THR:HG21	2:B:289:LYS:HD3	1.97	0.46
2:B:351:LEU:HA	2:B:352:PRO:HD3	1.71	0.46
2:D:373:PRO:O	2:D:374:GLU:C	2.52	0.46
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.30	0.46
1:A:286:PHE:O	1:A:287:GLN:C	2.52	0.46
2:D:425:ASN:ND2	4:D:2038:HOH:O	2.48	0.46
2:D:203:GLN:OE1	2:D:247:SER:HA	2.15	0.46
2:D:335:PHE:O	2:D:339:LEU:N	2.49	0.46
2:B:216:ASP:HB2	2:B:406:GLN:HG2	1.97	0.46
1:C:181:SER:O	1:C:182:THR:C	2.54	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.51	0.45
1:C:284:PRO:O	1:C:287:GLN:HG2	2.16	0.45
1:A:129:LYS:HD2	1:A:131:GLN:OE1	2.16	0.45
1:C:84:HIS:ND1	1:C:136:ASN:HA	2.30	0.45
2:B:203:GLN:HB3	2:B:206:ILE:HG12	1.96	0.45
1:C:216:PHE:CD1	1:C:222:PRO:HD3	2.52	0.45
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.51	0.45
1:C:37:LEU:HD11	1:C:76:LEU:HD22	1.98	0.45
2:B:220:GLU:HB2	3:E:88:VAL:HG13	1.99	0.45
1:A:227:TRP:O	1:A:230:VAL:HG22	2.17	0.45
2:D:210:MET:HE1	2:D:250:ARG:CB	2.46	0.45
1:A:10:ILE:HD12	1:A:20:LYS:HB2	1.98	0.45
1:C:50:ARG:O	1:C:54:LEU:HG	2.16	0.45
1:A:73:GLU:OE2	1:C:2:GLU:HG3	2.17	0.45
2:D:383:THR:N	2:D:386:SER:OG	2.49	0.45
2:D:401:ALA:C	2:D:403:GLN:N	2.69	0.45
2:D:211:ARG:HD3	2:D:344:ALA:HB2	1.99	0.45
2:D:332:LEU:HD23	2:D:363:ALA:CA	2.46	0.45
2:D:376:LEU:HD23	2:D:376:LEU:HA	1.83	0.45
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.99	0.45
1:A:291:LYS:HG2	1:A:291:LYS:O	2.16	0.45
2:B:200:MET:HB2	2:B:200:MET:HE2	1.83	0.45
1:C:68:ASP:OD1	1:C:69:VAL:N	2.49	0.45
2:B:175:VAL:C	2:B:179:HIS:CE1	2.91	0.44
2:D:401:ALA:C	2:D:403:GLN:H	2.20	0.44
2:B:384:LEU:HA	2:B:384:LEU:HD12	1.74	0.44
2:D:187:ARG:CZ	2:D:382:TYR:OH	2.65	0.44
2:D:303:THR:O	2:D:304:PHE:HB2	2.16	0.44
1:C:199:ARG:O	1:C:200:ARG:CB	2.65	0.44
1:C:227:TRP:CE3	1:C:269:TYR:HB3	2.53	0.44
1:A:157:ARG:NH2	2:B:228:GLN:HG3	2.32	0.44
2:B:411:GLU:O	2:B:412:LYS:C	2.55	0.44
1:A:217:ARG:HD3	1:A:243:TRP:CZ2	2.52	0.44
1:A:250:LYS:HD3	4:A:2062:HOH:O	2.17	0.44
1:C:57:GLU:O	1:C:58:LEU:C	2.55	0.44
2:D:315:LEU:O	2:D:316:THR:C	2.56	0.44
1:C:164:VAL:O	1:C:169:ARG:NH2	2.47	0.44
2:D:215:VAL:HB	2:D:342:ILE:HD13	2.00	0.44
2:B:326:ASN:O	2:B:329:VAL:HB	2.18	0.44
2:D:216:ASP:CG	2:D:408:SER:HG	2.21	0.44
2:D:360:PHE:HE2	2:D:376:LEU:HD12	1.79	0.43
2:D:361:HIS:C	2:D:363:ALA:N	2.70	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:THR:O	1:A:41:THR:N	2.50	0.43
1:C:248:PHE:HA	1:C:251:VAL:HB	2.00	0.43
1:A:278:LYS:NZ	2:B:181:ASP:OD2	2.51	0.43
1:C:216:PHE:C	1:C:218:THR:N	2.71	0.43
2:D:345:ASP:HA	2:D:346:PRO:HA	1.76	0.43
2:B:217:TRP:O	2:B:221:VAL:HG23	2.18	0.43
2:D:371:SER:O	2:D:372:TRP:C	2.55	0.43
1:A:44:VAL:HA	1:A:45:PRO:HD3	1.92	0.43
1:C:101:LEU:N	1:C:102:PRO:CD	2.81	0.43
2:D:202:LYS:O	2:D:204:PRO:HD3	2.18	0.43
1:A:129:LYS:HB2	1:A:130:PRO:HD2	2.00	0.43
1:C:88:LYS:HG3	1:C:131:GLN:HE22	1.76	0.43
2:D:402:PRO:HG3	2:D:410:ARG:NE	2.34	0.43
1:A:217:ARG:CG	1:A:243:TRP:CE2	3.02	0.43
1:A:101:LEU:N	1:A:102:PRO:HD3	2.33	0.43
2:B:207:THR:HB	4:B:2017:HOH:O	2.17	0.43
2:D:430:LEU:O	2:D:431:ASN:HB2	2.19	0.43
2:D:292:LEU:HA	2:D:292:LEU:HD12	1.72	0.43
1:A:290:THR:O	1:A:292:PRO:HD2	2.17	0.43
1:C:195:GLU:O	1:C:199:ARG:HA	2.18	0.43
2:D:343:ASP:HB3	2:D:345:ASP:O	2.19	0.43
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.54	0.42
2:D:205:ASP:O	2:D:205:ASP:OD1	2.37	0.42
2:B:388:LYS:O	2:B:392:MET:HG2	2.19	0.42
1:A:255:LEU:HD12	1:A:255:LEU:HA	1.69	0.42
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.54	0.42
2:D:389:PRO:O	2:D:392:MET:HB2	2.19	0.42
2:D:210:MET:CE	2:D:250:ARG:CB	2.95	0.42
1:C:99:ILE:HA	1:C:100:PRO:HD3	1.93	0.42
2:D:357:GLY:C	2:D:358:ALA:O	2.57	0.42
1:C:181:SER:O	1:C:183:ALA:N	2.52	0.42
1:A:15:TYR:N	4:A:2003:HOH:O	2.19	0.42
2:D:322:GLN:HB3	2:D:324:PRO:HD2	2.02	0.42
1:A:284:PRO:O	1:A:285:PHE:C	2.58	0.42
2:D:321:HIS:N	2:D:321:HIS:CD2	2.85	0.42
1:C:241:PRO:HB2	1:C:243:TRP:CZ3	2.54	0.42
2:D:425:ASN:HA	2:D:426:PRO:HD3	1.90	0.42
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.75	0.42
1:A:39:THR:O	1:A:41:THR:OG1	2.25	0.42
2:B:368:THR:CB	2:B:370:GLN:HE21	2.33	0.42
1:A:99:ILE:HA	1:A:100:PRO:HD3	1.86	0.42
1:A:97:THR:HA	4:A:2027:HOH:O	2.17	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:288:ASP:OD1	1:A:288:ASP:N	2.51	0.42
1:C:250:LYS:HD3	1:C:250:LYS:HA	1.96	0.42
2:B:233:HIS:HB3	2:B:310:THR:HB	2.02	0.42
1:C:283:HIS:HA	1:C:284:PRO:HD3	1.85	0.41
2:B:194:LYS:HA	2:B:195:PRO:HD3	1.60	0.41
2:B:351:LEU:HB3	2:B:352:PRO:CD	2.50	0.41
1:C:202:LEU:N	4:C:2032:HOH:O	2.52	0.41
1:A:25:LEU:O	2:D:294:MET:HE1	2.19	0.41
1:A:0:SER:HB2	1:A:1:MET:H	1.24	0.41
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.55	0.41
2:D:401:ALA:CB	2:D:402:PRO:CD	2.87	0.41
1:A:217:ARG:HG2	1:A:243:TRP:CG	2.55	0.41
2:D:176:PRO:C	2:D:178:TYR:N	2.74	0.41
2:D:415:ASN:OD1	2:D:417:LYS:HB3	2.20	0.41
2:D:392:MET:O	2:D:395:HIS:N	2.49	0.41
2:D:194:LYS:HA	2:D:195:PRO:HD3	1.90	0.41
1:A:163:VAL:O	1:A:164:VAL:HB	2.21	0.41
2:D:366:THR:HG23	2:D:427:PRO:HG3	2.01	0.41
2:B:371:SER:O	2:B:372:TRP:C	2.59	0.41
1:C:7:VAL:O	1:C:8:GLU:HB3	2.21	0.41
2:D:362:LEU:HD12	2:D:362:LEU:O	2.21	0.41
2:D:402:PRO:HG3	2:D:410:ARG:CZ	2.51	0.41
1:A:10:ILE:HD11	1:A:82:PHE:CE1	2.43	0.41
1:A:253:PRO:N	1:A:254:PRO:CD	2.84	0.41
1:A:122:ARG:HD2	1:A:122:ARG:O	2.20	0.41
1:C:55:LEU:HD11	1:C:146:PHE:CD1	2.56	0.41
1:C:1:MET:HE1	1:C:32:LEU:HD13	2.01	0.41
1:C:44:VAL:HB	1:C:49:ILE:HD11	2.02	0.41
1:A:209:ILE:HD11	1:A:213:PHE:CZ	2.56	0.41
2:D:339:LEU:HD23	2:D:339:LEU:HA	1.89	0.41
2:B:316:THR:HG21	4:B:2043:HOH:O	2.20	0.41
2:B:275:VAL:HG11	2:B:292:LEU:CD1	2.50	0.41
1:A:177:CYS:HB2	1:A:233:MET:CE	2.51	0.40
1:A:10:ILE:HG22	1:A:18:VAL:O	2.21	0.40
2:D:365:TYR:HA	2:D:370:GLN:O	2.21	0.40
1:C:175:LEU:HA	1:C:175:LEU:HD23	1.95	0.40
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.52	0.40
1:A:88:LYS:HA	1:A:91:MET:CE	2.51	0.40
1:C:233:MET:HA	1:C:234:PRO:HD3	1.90	0.40
1:C:221:THR:HA	1:C:222:PRO:HD3	1.84	0.40
1:C:84:HIS:CE1	1:C:135:ILE:HG13	2.56	0.40
2:B:289:LYS:HE3	2:B:293:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:283:HIS:ND1	1:C:284:PRO:CD	2.76	0.40
2:B:279:VAL:O	2:B:282:THR:OG1	2.39	0.40
1:A:41:THR:HB	1:A:42:GLU:H	1.40	0.40
2:B:190:GLU:OE1	2:B:352:PRO:HD2	2.22	0.40
1:A:33:LYS:CD	4:A:2009:HOH:O	2.69	0.40
1:C:65:LYS:HG2	1:C:67:LEU:HD23	2.02	0.40
1:C:155:PRO:O	1:C:156:VAL:C	2.60	0.40
2:D:324:PRO:O	2:D:325:ALA:C	2.60	0.40
1:C:78:LEU:HD23	1:C:78:LEU:N	2.37	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_456]	1.64	0.56

## 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	291/303 (96%)	266 (91%)	18 (6%)	7 (2%)	9	13
1	C	291/303 (96%)	253 (87%)	29 (10%)	9 (3%)	7	8
2	B	256/259 (99%)	242 (94%)	9 (4%)	5 (2%)	11	17
2	D	256/259 (99%)	229 (90%)	16 (6%)	11 (4%)	4	4
3	E	7/9 (78%)	4 (57%)	2 (29%)	1 (14%)	0	0
All	All	1101/1133 (97%)	994 (90%)	74 (7%)	33 (3%)	7	9

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
2	B	199	TYR
1	C	57	GLU

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Mol	Chain	Res	Type
1	C	199	ARG
2	D	358	ALA
2	D	359	ALA
1	A	40	GLU
1	A	97	THR
1	A	162	GLU
1	A	164	VAL
1	C	58	LEU
1	C	162	GLU
1	C	164	VAL
1	C	200	ARG
2	D	362	LEU
3	E	89	LYS
2	B	176	PRO
2	B	431	ASN
2	D	325	ALA
2	D	392	MET
1	A	208	GLU
1	C	40	GLU
1	C	145	ASP
2	D	372	TRP
2	D	393	ASP
2	D	421	VAL
1	A	291	LYS
2	B	284	ASP
2	B	389	PRO
2	D	402	PRO
1	C	230	VAL
2	D	176	PRO
2	D	401	ALA

### 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	258/265 (97%)	229 (89%)	29 (11%)	9	15
1	C	258/265 (97%)	231 (90%)	27 (10%)	10	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	232/233 (100%)	218 (94%)	14 (6%)	27	47
2	D	232/233 (100%)	207 (89%)	25 (11%)	9	17
3	E	9/9 (100%)	6 (67%)	3 (33%)	0	0
All	All	989/1005 (98%)	891 (90%)	98 (10%)	11	21

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	14	THR
1	A	40	GLU
1	A	41	THR
1	A	49	ILE
1	A	55	LEU
1	A	59	ASN
1	A	71	HIS
1	A	74	ASN
1	A	75	LYS
1	A	83	LEU
1	A	97	THR
1	A	101	LEU
1	A	122	ARG
1	A	129	LYS
1	A	150	ARG
1	A	157	ARG
1	A	178	LYS
1	A	200	ARG
1	A	206	ASP
1	A	209	ILE
1	A	226	VAL
1	A	230	VAL
1	A	237	LYS
1	A	238	PRO
1	A	248	PHE
1	A	255	LEU
1	A	256	ASP
1	A	261	SER
2	B	175	VAL
2	B	180	GLU
2	B	196	LYS
2	B	199	TYR

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Mol	Chain	Res	Type
2	B	232	LEU
2	B	245	SER
2	B	281	ILE
2	B	316	THR
2	B	328	LYS
2	B	334	MET
2	B	348	LEU
2	B	384	LEU
2	B	417	LYS
2	B	428	GLU
1	C	0	SER
1	C	9	LYS
1	C	10	ILE
1	C	15	TYR
1	C	22	ARG
1	C	42	GLU
1	C	55	LEU
1	C	57	GLU
1	C	71	HIS
1	C	72	THR
1	C	73	GLU
1	C	76	LEU
1	C	88	LYS
1	C	101	LEU
1	C	122	ARG
1	C	150	ARG
1	C	155	PRO
1	C	163	VAL
1	C	177	CYS
1	C	189	LEU
1	C	206	ASP
1	C	217	ARG
1	C	226	VAL
1	C	248	PHE
1	C	249	SER
1	C	276	SER
1	C	278	LYS
2	D	179	HIS
2	D	180	GLU
2	D	196	LYS
2	D	210	MET
2	D	232	LEU

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Mol	Chain	Res	Type
2	D	245	SER
2	D	250	ARG
2	D	261	MET
2	D	277	GLU
2	D	283	ASP
2	D	284	ASP
2	D	285	THR
2	D	292	LEU
2	D	316	THR
2	D	334	MET
2	D	335	PHE
2	D	348	LEU
2	D	370	GLN
2	D	371	SER
2	D	391	LEU
2	D	403	GLN
2	D	415	ASN
2	D	425	ASN
2	D	429	THR
2	D	432	LEU
3	E	88	VAL
3	E	91	ARG
3	E	94	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	119	HIS
1	A	131	GLN
1	A	268	HIS
2	B	179	HIS
2	B	183	HIS
2	B	296	HIS
2	B	313	GLN
2	B	395	HIS
2	B	396	GLN
2	B	403	GLN
2	B	425	ASN
1	C	60	HIS
1	C	71	HIS
1	C	131	GLN

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Mol	Chain	Res	Type
1	C	268	HIS
2	D	254	GLN
2	D	321	HIS
2	D	361	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	5.84	4 (40%)	12,14,16	1.37	1 (8%)
1	TPO	C	160	1	10,10,11	4.94	3 (30%)	12,14,16	0.89	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	-	0/9/11/13	0/0/0/0
1	TPO	C	160	1	-	0/9/11/13	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	O-C	17.71	1.23	1.11
1	C	160	TPO	O-C	14.85	1.21	1.11
1	C	160	TPO	P-OG1	-3.60	1.48	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-OG1	-3.56	1.48	1.59
1	C	160	TPO	OG1-CB	-2.18	1.41	1.45
1	A	160	TPO	CA-C	2.06	1.52	1.48
1	A	160	TPO	OG1-CB	-2.02	1.41	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O2P-P-OG1	2.59	114.55	107.09

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	294/303 (97%)	0.03	10 (3%) 43 44	25, 38, 80, 119	0
1	C	294/303 (97%)	0.78	51 (17%) 2 2	31, 54, 209, 228	0
2	B	258/259 (99%)	0.04	10 (3%) 37 38	25, 37, 61, 87	0
2	D	258/259 (99%)	0.74	42 (16%) 2 2	26, 56, 132, 186	0
3	E	9/9 (100%)	1.32	1 (11%) 6 6	49, 57, 78, 97	0
All	All	1113/1133 (98%)	0.41	114 (10%) 7 7	25, 45, 121, 228	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	TYR	9.8
2	D	432	LEU	8.7
1	C	249	SER	8.5
1	A	40	GLU	7.6
1	C	225	VAL	7.1
1	C	250	LYS	6.7
3	E	95	GLU	6.3
1	C	240	PHE	5.8
1	C	226	VAL	5.8
1	C	243	TRP	5.3
1	C	241	PRO	5.3
2	D	323	GLN	5.2
1	A	95	ALA	5.1
2	D	284	ASP	5.1
1	C	236	TYR	5.0
1	C	245	ARG	5.0
1	A	39	THR	4.9
1	C	247	ASP	4.9
1	C	233	MET	4.8
1	C	14	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	230	VAL	4.4
1	C	237	LYS	4.3
1	C	223	ASP	4.3
1	A	96	LEU	4.3
1	C	227	TRP	4.3
2	D	430	LEU	4.2
1	C	228	PRO	4.2
2	B	324	PRO	4.0
1	C	179	TYR	4.0
1	A	38	ASP	3.9
2	B	429	THR	3.8
2	D	324	PRO	3.8
2	D	431	ASN	3.8
1	C	239	SER	3.7
2	D	417	LYS	3.7
2	D	311	VAL	3.6
1	C	273	LYS	3.5
2	D	383	THR	3.5
2	D	325	ALA	3.5
2	D	388	LYS	3.5
1	C	189	LEU	3.4
2	D	423	LEU	3.4
2	B	323	GLN	3.4
1	C	231	THR	3.4
2	B	431	ASN	3.4
2	B	176	PRO	3.4
2	D	176	PRO	3.3
2	B	403	GLN	3.3
1	C	238	PRO	3.2
2	D	177	ASP	3.2
2	D	283	ASP	3.2
2	D	416	SER	3.2
2	D	415	ASN	3.2
1	C	178	LYS	3.1
1	C	17	VAL	3.1
1	C	293	VAL	3.1
1	C	244	ALA	3.1
1	C	224	GLU	3.0
1	C	36	ARG	3.0
1	C	192	ILE	3.0
2	D	365	TYR	3.0
1	C	287	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	162	GLU	3.0
1	A	178	LYS	2.9
1	C	248	PHE	2.9
2	D	419	HIS	2.9
2	D	385	GLU	2.9
2	D	320	LEU	2.9
1	C	9	LYS	2.8
2	B	201	LYS	2.8
1	C	162	GLU	2.8
2	D	271	TYR	2.8
1	C	187	TRP	2.8
2	D	328	LYS	2.8
2	D	428	GLU	2.7
2	D	355	ILE	2.7
2	D	280	TYR	2.7
1	C	191	CYS	2.6
1	C	175	LEU	2.6
2	D	334	MET	2.6
2	D	399	LEU	2.5
1	C	188	SER	2.5
2	D	202	LYS	2.5
2	D	233	HIS	2.5
2	D	427	PRO	2.4
1	C	137	THR	2.4
1	C	128	LEU	2.4
2	D	335	PHE	2.4
1	C	246	GLN	2.3
2	B	428	GLU	2.3
2	D	337	GLY	2.3
2	D	327	CYS	2.2
2	D	403	GLN	2.2
1	C	200	ARG	2.2
1	C	253	PRO	2.2
1	C	257	GLU	2.2
1	C	13	GLY	2.2
2	D	359	ALA	2.2
2	D	226	LYS	2.2
2	D	381	GLY	2.1
2	B	236	VAL	2.1
1	A	0	SER	2.1
2	D	418	TYR	2.1
1	C	158	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	206	ASP	2.1
1	C	288	ASP	2.1
2	D	424	LEU	2.1
2	B	337	GLY	2.1
1	C	0	SER	2.0
1	C	232	SER	2.0
2	D	340	SER	2.0
2	D	386	SER	2.0
1	A	73	GLU	2.0
1	C	161	HIS	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	0.12	-0.64	29,37,46,48	0
1	TPO	C	160	11/12	0.15	-0.67	43,51,58,60	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.