



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:46 PM 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 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

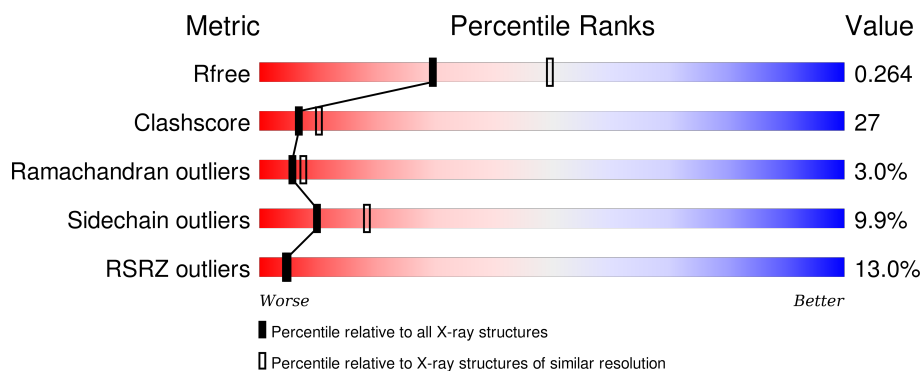
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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>5%</div> <div> <div>54%</div> <div>34%</div> <div>8%</div> <div>••</div> </div> </div>
1	C	303	<div> <div>20%</div> <div> <div>45%</div> <div>42%</div> <div>11%</div> <div>•</div> </div> </div>
2	B	259	<div> <div>7%</div> <div> <div>65%</div> <div>30%</div> <div>5%</div> </div> </div>
2	D	259	<div> <div>19%</div> <div> <div>53%</div> <div>36%</div> <div>10%</div> <div>•</div> </div> </div>
3	E	9	<div> <div>22%</div> <div> <div>11%</div> <div>56%</div> <div>33%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9201 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 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			

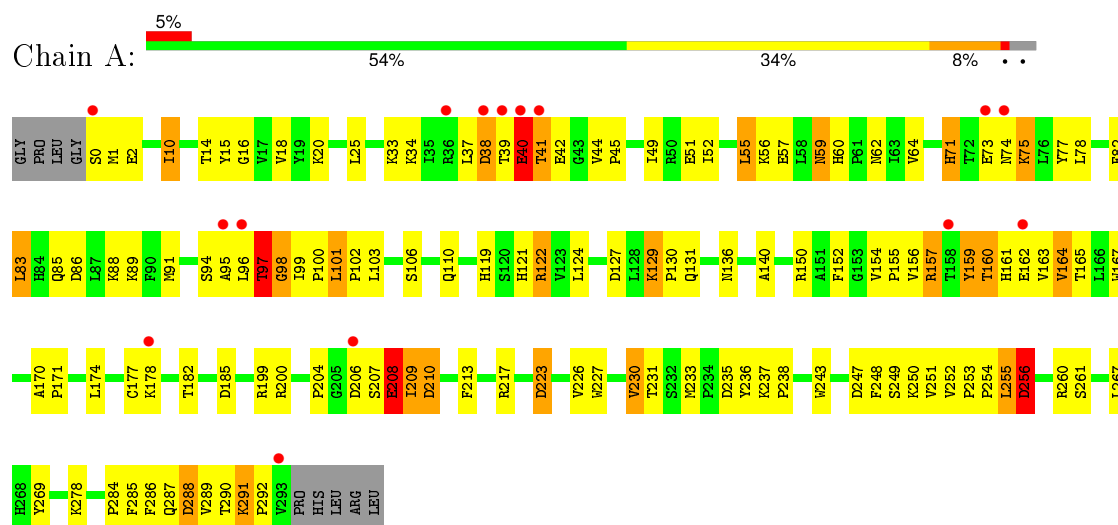
- Molecule 4 is water.

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		

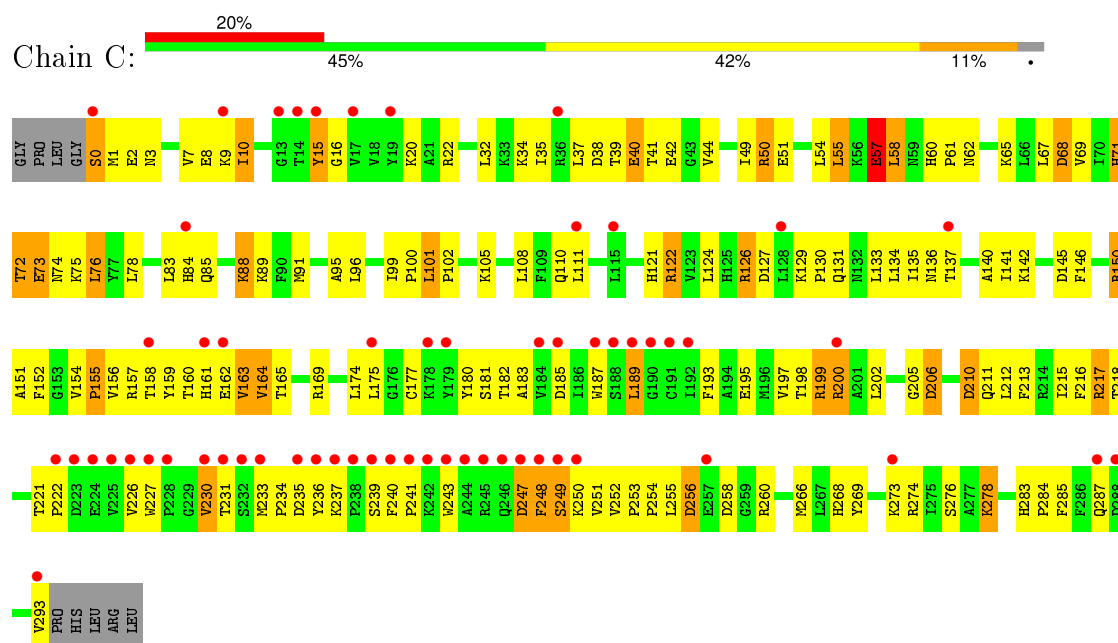
### 3 Residue-property plots [i](#)

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.

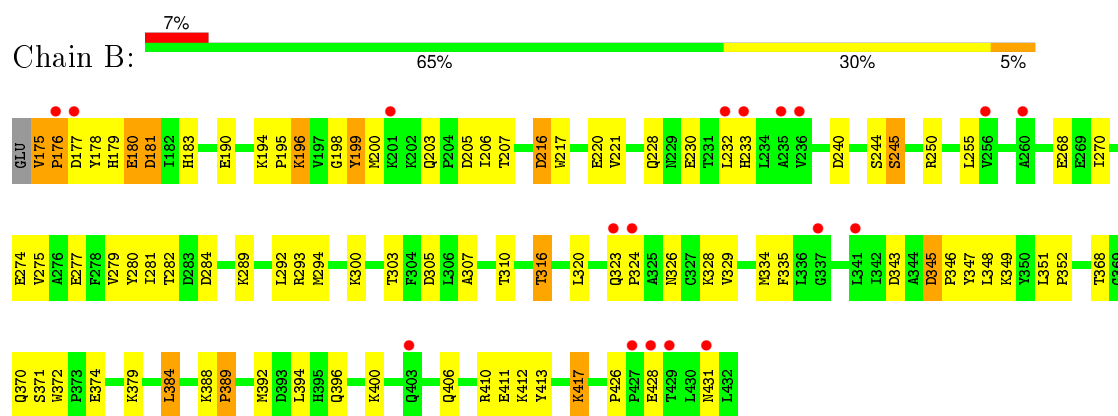
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



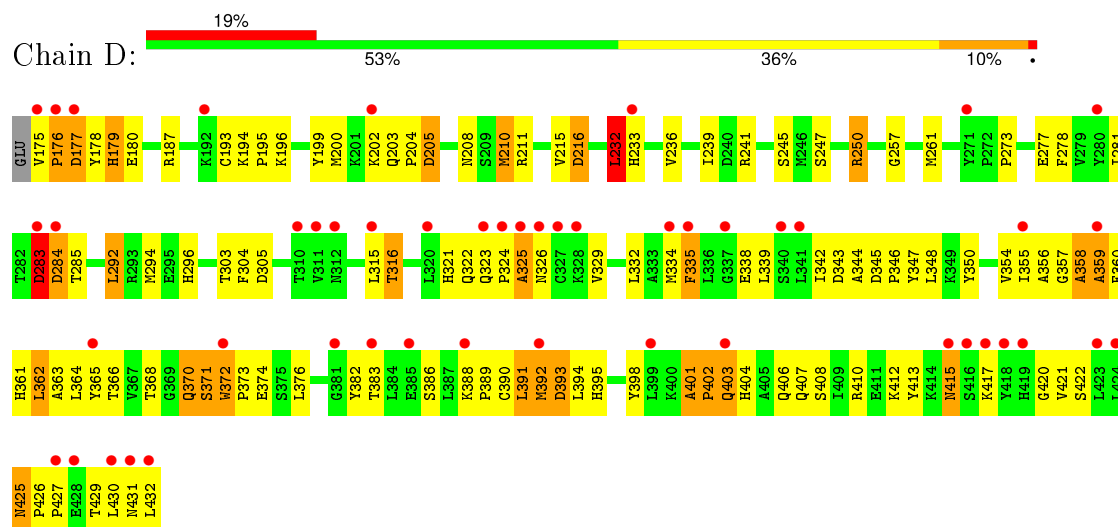
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



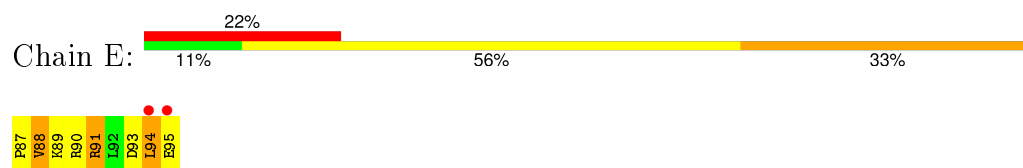
#### • Molecule 2: CYCLIN A2



• Molecule 2: CYCLIN A2



• Molecule 3: TRANSCRIPTION FACTOR E2F1



## 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 , 0.264	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> )	0.39 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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.

<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

### 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	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 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 27.

All (488) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.65	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:NH2	2:B:374:GLU:OE2[4_456]	1.64	0.56

## 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	291/303 (96%)	266 (91%)	18 (6%)	7 (2%)	<b>7</b> <b>11</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	291/303 (96%)	253 (87%)	29 (10%)	9 (3%)	5	7
2	B	256/259 (99%)	242 (94%)	9 (4%)	5 (2%)	9	15
2	D	256/259 (99%)	229 (90%)	16 (6%)	11 (4%)	3	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%)	5	7

All (33) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	7	14
1	C	258/265 (97%)	231 (90%)	27 (10%)	8	16
2	B	232/233 (100%)	218 (94%)	14 (6%)	24	43
2	D	232/233 (100%)	207 (89%)	25 (11%)	8	15
3	E	9/9 (100%)	6 (67%)	3 (33%)	0	0
All	All	989/1005 (98%)	891 (90%)	98 (10%)	10	18

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
1	C	268	HIS
2	D	254	GLN
2	D	321	HIS
2	D	361	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	TPO	A	160	1	8,10,11	1.63	1 (12%)	7,14,16	1.43	2 (28%)
1	TPO	C	160	1	8,10,11	1.55	1 (12%)	7,14,16	1.50	1 (14%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	-3.71	1.48	1.60
1	A	160	TPO	P-OG1	-3.67	1.48	1.60

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O-C-CA	-2.89	117.81	125.44
1	A	160	TPO	O-C-CA	-2.62	118.51	125.44
1	A	160	TPO	OG1-P-O1P	-2.07	101.95	107.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	160	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

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	293/303 (96%)	0.15	15 (5%) 32 36	25, 38, 80, 119	0
1	C	293/303 (96%)	0.96	60 (20%) 1 1	31, 54, 209, 228	0
2	B	258/259 (99%)	0.19	18 (6%) 19 22	25, 37, 61, 87	0
2	D	258/259 (99%)	0.92	49 (18%) 2 1	26, 56, 132, 186	0
3	E	9/9 (100%)	1.51	2 (22%) 1 1	49, 57, 78, 97	0
All	All	1111/1133 (98%)	0.56	144 (12%) 5 4	25, 45, 121, 228	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	SER	10.8
1	C	15	TYR	10.3
2	D	432	LEU	9.7
1	C	226	VAL	8.7
1	A	40	GLU	8.1
1	C	225	VAL	7.7
3	E	95	GLU	6.7
1	A	95	ALA	6.4
1	C	250	LYS	6.2
1	C	236	TYR	6.2
1	C	245	ARG	5.8
2	D	323	GLN	5.5
1	C	227	TRP	5.4
2	D	284	ASP	5.4
1	C	247	ASP	5.4
1	C	14	THR	5.3
2	D	430	LEU	5.3
1	C	243	TRP	5.2
1	C	241	PRO	5.1
1	C	237	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	230	VAL	5.1
2	B	324	PRO	5.0
1	C	240	PHE	5.0
1	A	96	LEU	4.9
1	C	179	TYR	4.8
1	A	39	THR	4.8
1	C	233	MET	4.8
2	D	311	VAL	4.7
1	C	228	PRO	4.7
1	C	223	ASP	4.5
2	D	431	ASN	4.5
2	B	429	THR	4.5
1	A	38	ASP	4.4
2	B	176	PRO	4.4
1	C	189	LEU	4.2
2	D	388	LYS	4.2
2	D	176	PRO	4.2
2	D	324	PRO	4.2
1	C	231	THR	4.2
1	C	248	PHE	4.0
2	D	177	ASP	3.9
1	C	239	SER	3.8
1	C	273	LYS	3.8
2	D	417	LYS	3.8
1	C	238	PRO	3.8
2	D	327	CYS	3.7
2	D	419	HIS	3.6
2	D	383	THR	3.6
2	D	320	LEU	3.6
1	C	36	ARG	3.5
2	D	283	ASP	3.5
1	C	175	LEU	3.5
1	C	128	LEU	3.5
2	B	323	GLN	3.5
2	B	403	GLN	3.4
2	D	423	LEU	3.4
2	D	325	ALA	3.4
1	C	17	VAL	3.4
1	A	162	GLU	3.3
2	B	431	ASN	3.3
2	D	415	ASN	3.3
1	C	192	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	416	SER	3.2
2	D	365	TYR	3.2
1	C	191	CYS	3.2
1	C	162	GLU	3.2
1	C	178	LYS	3.1
1	C	232	SER	3.1
2	D	355	ILE	3.1
1	C	187	TRP	3.1
1	C	293	VAL	3.1
2	D	233	HIS	3.1
2	D	271	TYR	3.0
1	C	9	LYS	3.0
2	D	428	GLU	3.0
2	B	236	VAL	2.9
2	B	201	LYS	2.9
1	C	13	GLY	2.9
1	A	178	LYS	2.9
2	D	334	MET	2.9
1	C	158	THR	2.9
2	D	399	LEU	2.8
1	C	244	ALA	2.8
1	C	137	THR	2.7
1	C	188	SER	2.7
2	D	424	LEU	2.7
1	C	287	GLN	2.7
2	B	232	LEU	2.7
2	D	280	TYR	2.7
1	C	224	GLU	2.6
2	D	337	GLY	2.6
1	C	257	GLU	2.6
1	C	190	GLY	2.6
2	D	385	GLU	2.6
2	D	427	PRO	2.6
1	C	222	PRO	2.6
2	D	328	LYS	2.6
2	D	202	LYS	2.6
2	D	403	GLN	2.6
1	C	115	LEU	2.5
2	B	428	GLU	2.5
1	C	200	ARG	2.5
1	C	161	HIS	2.5
2	D	359	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	326	ASN	2.5
2	B	177	ASP	2.5
1	A	74	ASN	2.4
2	B	337	GLY	2.4
1	C	111	LEU	2.4
2	D	175	VAL	2.4
2	D	335	PHE	2.4
1	A	41	THR	2.4
1	C	246	GLN	2.4
2	D	381	GLY	2.4
1	A	73	GLU	2.3
2	D	192	LYS	2.3
1	A	36	ARG	2.3
2	B	260	ALA	2.3
2	B	341	LEU	2.3
2	D	418	TYR	2.3
1	C	84	HIS	2.2
2	D	340	SER	2.2
2	B	235	ALA	2.2
3	E	94	LEU	2.2
2	D	310	THR	2.2
2	D	341	LEU	2.2
1	A	293	VAL	2.2
1	C	19	TYR	2.1
1	A	158	THR	2.1
2	B	233	HIS	2.1
2	D	372	TRP	2.1
1	C	185	ASP	2.1
2	D	392	MET	2.1
2	D	315	LEU	2.1
1	A	206	ASP	2.1
2	B	256	VAL	2.1
1	C	0	SER	2.1
2	B	427	PRO	2.0
1	C	288	ASP	2.0
1	C	242	LYS	2.0
2	D	312	ASN	2.0
1	C	184	VAL	2.0
1	C	235	ASP	2.0
1	A	0	SER	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( $\text{\AA}^2$ )	Q<0.9
1	TPO	C	160	11/12	0.96	0.17	-	43,51,58,60	0
1	TPO	A	160	11/12	0.99	0.14	-	29,37,46,48	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.