



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:46 PM GMT

PDB ID : 1H27  
Title : CDK2/CYCLIN A IN COMPLEX WITH AN 11-RESIDUE RECRUITMENT PEPTIDE FROM P27  
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 : 2.20 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

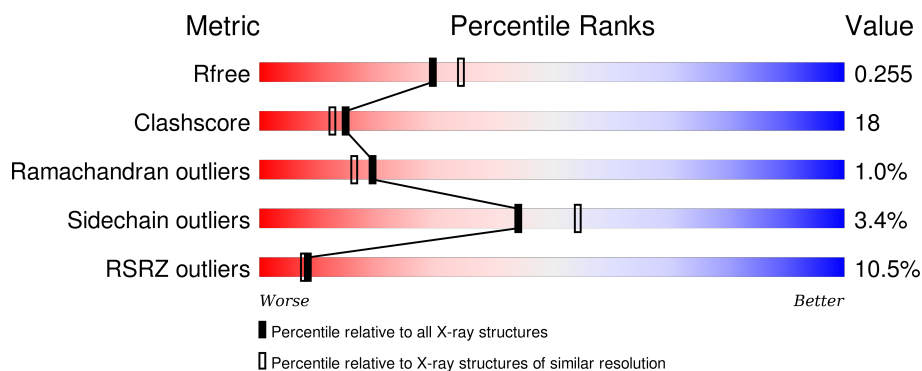
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	<div> <div>7%</div> <div>69%</div> <div>27%</div> <div>• •</div> </div>
1	C	303	<div> <div>14%</div> <div>63%</div> <div>30%</div> <div>• •</div> </div>
2	B	259	<div> <div>5%</div> <div>77%</div> <div>20%</div> <div>•</div> </div>
2	D	259	<div> <div>14%</div> <div>62%</div> <div>35%</div> <div>•</div> </div>
3	E	11	<div> <div>45%</div> <div>36%</div> <div>18%</div> <div>45%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9182 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	298	Total	C	N	O	P	S	9	0	1
			2389	1550	405	425	1	8			
1	C	293	Total	C	N	O	P	S	0	0	1
			2342	1516	398	419	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
			2084	1350	339	384	11			
2	D	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			

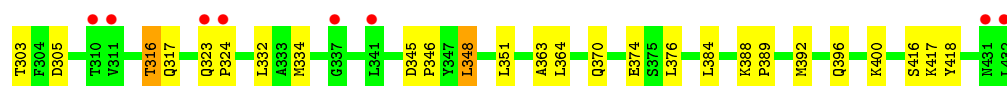
- Molecule 3 is a protein called CYCLIN-DEPENDENT KINASE INHIBITOR 1B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			50	32	10	8			

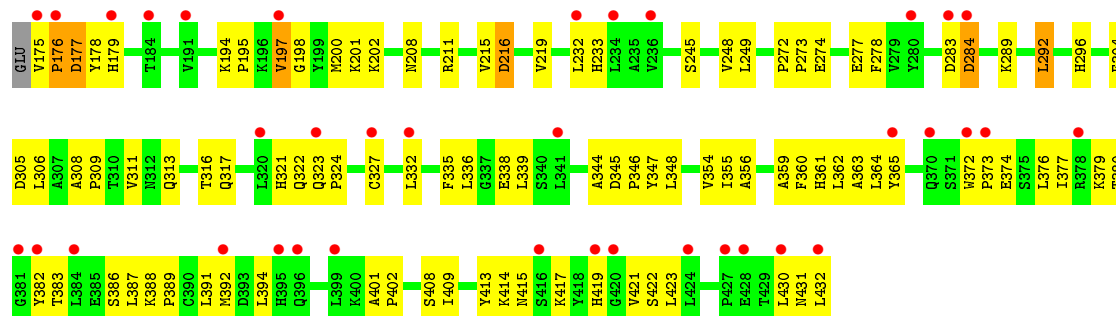
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	75	Total	O	0	0
			75	75		
4	C	45	Total	O	0	0
			45	45		
4	D	26	Total	O	0	0
			26	26		

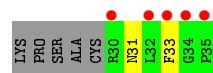




● Molecule 2: CYCLIN A2



● Molecule 3: CYCLIN-DEPENDENT KINASE INHIBITOR 1B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.69Å 133.55Å 148.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 2.20 33.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.75-2.20) 98.7 (33.88-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.227 , 0.269 0.229 , 0.255	Depositor DCC
$R_{free}$ test set	3715 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.5	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 73895 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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	0.87	0/2439	0.88	6/3310 (0.2%)
1	C	0.72	1/2387 (0.0%)	0.81	7/3237 (0.2%)
2	B	0.87	0/2134	0.85	5/2897 (0.2%)
2	D	0.66	0/2134	0.75	4/2897 (0.1%)
3	E	0.35	0/51	0.43	0/66
All	All	0.78	1/9145 (0.0%)	0.82	22/12407 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	79	VAL	CB-CG1	5.18	1.63	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	305	ASP	CB-CG-OD2	7.83	125.35	118.30
1	A	256	ASP	CB-CG-OD2	7.59	125.13	118.30
2	D	305	ASP	CB-CG-OD2	6.91	124.52	118.30
2	B	283	ASP	CB-CG-OD2	6.78	124.40	118.30
1	C	127	ASP	CB-CG-OD2	6.73	124.36	118.30
1	A	270	ASP	CB-CG-OD2	6.42	124.07	118.30
1	C	68	ASP	CB-CG-OD2	6.33	124.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ASP	CB-CG-OD2	6.30	123.97	118.30
2	D	216	ASP	CB-CG-OD2	6.21	123.89	118.30
2	B	177	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	210	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	145	ASP	CB-CG-OD2	5.75	123.47	118.30
1	C	210	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	38	ASP	CB-CG-OD2	5.69	123.42	118.30
2	D	284	ASP	CB-CG-OD2	5.67	123.41	118.30
1	C	247	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	235	ASP	CB-CG-OD2	5.38	123.14	118.30
2	B	284	ASP	CB-CG-OD2	5.32	123.08	118.30
1	C	223	ASP	CB-CG-OD2	5.30	123.07	118.30
2	D	283	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	38	ASP	CB-CG-OD2	5.12	122.91	118.30
2	B	240	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	2389	0	2430	103	0
1	C	2342	0	2385	103	0
2	B	2084	0	2107	61	0
2	D	2084	0	2107	85	0
3	E	50	0	48	3	0
4	A	87	0	0	13	0
4	B	75	0	0	6	0
4	C	45	0	0	3	0
4	D	26	0	0	2	0
All	All	9182	0	9077	320	0



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 18.

All (320) 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)
2:B:177:ASP:HB2	4:B:2008:HOH:O	1.48	1.13
1:A:230:VAL:HA	1:A:233:MET:HE2	1.34	1.04
1:C:71:HIS:CD2	2:D:296:HIS:HE1	1.76	1.02
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.79	1.00
1:A:71:HIS:NE2	2:B:296:HIS:NE2	2.11	0.98
2:B:199:TYR:HA	2:B:202:LYS:HE2	1.50	0.94
1:A:71:HIS:NE2	2:B:296:HIS:CD2	2.36	0.92
2:D:388:LYS:HG3	2:D:432:LEU:HD13	1.53	0.91
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.40	0.90
1:A:106:SER:HB2	1:A:290:THR:O	1.71	0.89
1:A:154:VAL:O	2:B:316:THR:CG2	2.20	0.89
1:C:284:PRO:HA	1:C:287:GLN:HG2	1.56	0.88
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.55	0.88
1:A:154:VAL:O	2:B:316:THR:HG22	1.75	0.86
1:C:60:HIS:HD2	1:C:62:ASN:H	1.23	0.86
1:C:39:THR:N	4:C:2012:HOH:O	1.87	0.85
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.59	0.82
2:D:284:ASP:N	4:D:2021:HOH:O	2.05	0.82
1:A:39:THR:HG21	2:B:289:LYS:NZ	1.94	0.82
1:C:38:ASP:O	1:C:39:THR:CB	2.25	0.82
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.61	0.82
2:B:175:VAL:N	2:B:179:HIS:CE1	2.48	0.81
1:A:71:HIS:CD2	2:B:296:HIS:NE2	2.49	0.80
1:C:37:LEU:O	1:C:38:ASP:HB2	1.81	0.79
1:C:60:HIS:CD2	1:C:62:ASN:H	2.00	0.79
1:A:163:VAL:HG23	4:A:2021:HOH:O	1.81	0.79
2:D:197:VAL:HG13	2:D:198:GLY:N	1.98	0.78
1:C:38:ASP:O	1:C:39:THR:OG1	2.03	0.77
1:A:230:VAL:HA	1:A:233:MET:CE	2.15	0.76
1:A:294:PRO:C	1:A:296:LEU:H	1.86	0.76
1:C:126:ARG:HD2	1:C:163:VAL:HG21	1.68	0.75
1:C:64:VAL:HG23	1:C:143:LEU:O	1.87	0.75
2:D:313:GLN:O	2:D:316:THR:HG22	1.87	0.74
1:C:64:VAL:CG2	1:C:144:ALA:HB2	2.16	0.74
2:D:387:LEU:O	2:D:391:LEU:HB2	1.86	0.74
1:C:256:ASP:O	1:C:260:ARG:HG3	1.87	0.74
1:C:223:ASP:H	1:C:226:VAL:HG12	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:TPO:O2P	1:C:160:TPO:N	2.16	0.73
1:A:107:TYR:OH	1:A:135:ILE:HD13	1.88	0.73
1:A:39:THR:HG21	2:B:289:LYS:CD	2.19	0.72
1:A:148:LEU:HD12	4:A:2027:HOH:O	1.90	0.71
2:D:322:GLN:HG2	2:D:324:PRO:O	1.90	0.70
1:A:230:VAL:CA	1:A:233:MET:HE2	2.17	0.69
1:C:39:THR:O	1:C:40:GLU:HB2	1.93	0.68
1:C:84:HIS:CD2	1:C:85:GLN:HG2	2.28	0.68
2:B:175:VAL:N	2:B:179:HIS:HE1	1.90	0.68
1:A:51:GLU:O	1:A:55:LEU:HB2	1.94	0.68
1:C:227:TRP:CE3	1:C:269:TYR:HB3	2.29	0.67
1:A:60:HIS:CD2	1:A:62:ASN:H	2.13	0.67
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.60	0.66
1:C:252:VAL:HG11	1:C:255:LEU:HD22	1.78	0.66
1:C:12:GLU:HG3	1:C:16:GLY:O	1.96	0.66
1:C:154:VAL:O	2:D:316:THR:HG23	1.96	0.66
1:C:230:VAL:HA	1:C:233:MET:HE3	1.78	0.65
2:B:203:GLN:O	4:B:2018:HOH:O	2.14	0.65
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.62	0.65
1:A:223:ASP:H	1:A:226:VAL:HG12	1.62	0.65
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.77	0.64
2:D:321:HIS:CE1	2:D:379:LYS:HD2	2.33	0.64
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.79	0.64
1:A:296:LEU:CD1	4:A:2006:HOH:O	2.45	0.64
2:D:201:LYS:C	2:D:201:LYS:HD3	2.18	0.64
2:D:413:TYR:O	2:D:422:SER:OG	2.14	0.63
2:D:389:PRO:O	2:D:392:MET:HB2	1.99	0.63
1:A:97:THR:HG23	1:A:97:THR:O	1.99	0.62
2:B:293:ARG:HD3	1:C:2:GLU:OE1	1.99	0.62
1:C:155:PRO:HD2	2:D:316:THR:OG1	1.99	0.61
1:A:161:HIS:HD2	4:A:2009:HOH:O	1.81	0.61
4:A:2045:HOH:O	2:B:175:VAL:HG22	2.00	0.61
1:A:2:GLU:OE1	1:C:73:GLU:OE2	2.17	0.61
2:D:197:VAL:CG1	2:D:198:GLY:N	2.64	0.60
2:D:346:PRO:HD2	2:D:347:TYR:CD2	2.36	0.60
1:C:230:VAL:HA	1:C:233:MET:CE	2.30	0.60
2:B:210:MET:HB3	3:E:33:PHE:CE2	2.36	0.60
2:B:175:VAL:HG23	2:B:175:VAL:O	2.02	0.60
1:A:294:PRO:C	1:A:296:LEU:N	2.54	0.60
1:A:39:THR:HG21	2:B:289:LYS:HD2	1.83	0.60
2:D:197:VAL:HG13	2:D:198:GLY:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:LEU:HD23	3:E:33:PHE:CZ	2.38	0.59
1:C:39:THR:CA	4:C:2012:HOH:O	2.40	0.59
1:A:71:HIS:NE2	2:B:296:HIS:CG	2.71	0.59
1:C:39:THR:O	1:C:40:GLU:CB	2.49	0.59
1:C:129:LYS:HG3	1:C:131:GLN:HG2	1.83	0.59
1:C:252:VAL:HG12	1:C:255:LEU:HB2	1.84	0.59
1:C:64:VAL:HG21	1:C:144:ALA:CB	2.30	0.58
1:C:38:ASP:C	1:C:39:THR:OG1	2.41	0.58
1:A:154:VAL:O	2:B:316:THR:HG23	2.04	0.58
1:C:84:HIS:HD2	1:C:85:GLN:HG2	1.69	0.58
1:A:39:THR:HG22	1:A:40:GLU:H	1.69	0.57
2:B:396:GLN:HB3	2:B:400:LYS:HE2	1.87	0.57
1:A:88:LYS:C	1:A:90:PHE:H	2.08	0.57
2:D:373:PRO:O	2:D:377:ILE:HG13	2.05	0.57
1:A:60:HIS:HD2	1:A:62:ASN:H	1.50	0.57
1:A:296:LEU:HD12	4:A:2006:HOH:O	2.03	0.57
1:C:38:ASP:O	1:C:39:THR:HB	2.04	0.56
2:B:275:VAL:HG11	2:B:292:LEU:HD11	1.86	0.56
1:C:162:GLU:CD	1:C:162:GLU:H	2.08	0.56
1:A:260:ARG:HD3	4:A:2067:HOH:O	2.05	0.56
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.32	0.56
1:C:121:HIS:O	1:C:122:ARG:HG3	2.06	0.56
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.41	0.56
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.87	0.56
2:B:274:GLU:HG2	2:B:277:GLU:HG3	1.87	0.56
1:A:101:LEU:N	1:A:102:PRO:CD	2.68	0.56
1:A:288:ASP:HB3	4:A:2085:HOH:O	2.04	0.55
1:A:230:VAL:HG12	1:A:233:MET:HE2	1.88	0.55
2:D:233:HIS:HD2	4:D:2024:HOH:O	1.89	0.55
1:A:290:THR:C	1:A:292:PRO:HD3	2.26	0.55
1:C:230:VAL:HG23	1:C:231:THR:H	1.71	0.55
4:A:2045:HOH:O	2:B:175:VAL:CG2	2.55	0.55
2:B:233:HIS:HD2	4:B:2042:HOH:O	1.89	0.55
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.87	0.54
1:A:39:THR:HG21	2:B:289:LYS:CE	2.37	0.54
1:C:52:ILE:CD1	1:C:78:LEU:HD21	2.35	0.54
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.88	0.54
1:A:56:LYS:NZ	2:B:303:THR:O	2.40	0.54
1:C:262:LEU:HG	1:C:266:MET:HE2	1.89	0.54
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.88	0.54
2:D:415:ASN:OD1	2:D:417:LYS:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:HG22	1:A:104:ILE:HG13	1.90	0.53
1:A:39:THR:C	1:A:41:THR:H	2.12	0.53
2:D:389:PRO:O	2:D:392:MET:N	2.41	0.53
2:D:176:PRO:HA	2:D:179:HIS:CE1	2.44	0.53
1:C:129:LYS:HB2	1:C:130:PRO:HD2	1.90	0.53
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.36	0.53
2:B:288:LYS:O	2:B:292:LEU:HD13	2.08	0.53
1:C:40:GLU:OE2	2:D:289:LYS:NZ	2.43	0.52
1:C:262:LEU:HG	1:C:266:MET:CE	2.39	0.52
1:A:39:THR:HG21	2:B:289:LYS:HZ2	1.71	0.52
1:A:39:THR:HG22	1:A:40:GLU:N	2.24	0.52
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.92	0.52
2:D:414:LYS:HE2	2:D:423:LEU:HD21	1.92	0.52
1:C:83:LEU:HD23	1:C:136:ASN:HB3	1.92	0.51
1:C:223:ASP:H	1:C:226:VAL:CG1	2.20	0.51
1:C:219:LEU:O	1:C:220:GLY:O	2.27	0.51
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.69	0.51
1:C:61:PRO:O	1:C:142:LYS:HE2	2.11	0.51
1:C:284:PRO:CA	1:C:287:GLN:HG2	2.36	0.51
1:A:295:HIS:O	1:A:296:LEU:CB	2.59	0.50
1:C:10:ILE:HD11	1:C:20:LYS:HB2	1.94	0.50
2:D:175:VAL:N	2:D:176:PRO:HD3	2.27	0.50
1:C:74:ASN:ND2	4:C:2025:HOH:O	2.45	0.50
1:A:253:PRO:N	1:A:254:PRO:CD	2.75	0.50
2:D:361:HIS:O	2:D:362:LEU:C	2.50	0.50
1:C:7:VAL:O	1:C:8:GLU:HB3	2.12	0.50
1:A:227:TRP:HB3	1:A:230:VAL:HG13	1.93	0.50
1:C:91:MET:HE2	1:C:130:PRO:HB3	1.93	0.50
1:C:231:THR:HA	1:C:236:TYR:CD1	2.47	0.50
2:D:211:ARG:HD3	2:D:344:ALA:HB2	1.94	0.50
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.42	0.50
1:A:88:LYS:C	1:A:90:PHE:N	2.65	0.50
2:D:430:LEU:O	2:D:431:ASN:HB2	2.12	0.50
1:A:119:HIS:HD2	4:B:2009:HOH:O	1.95	0.50
1:A:296:LEU:HD11	4:A:2006:HOH:O	2.08	0.49
1:C:230:VAL:HG23	1:C:231:THR:N	2.26	0.49
1:C:219:LEU:HB2	1:C:269:TYR:OH	2.12	0.49
1:A:148:LEU:HB3	4:A:2027:HOH:O	2.12	0.49
1:C:121:HIS:C	1:C:122:ARG:HG3	2.33	0.49
2:D:197:VAL:CG1	2:D:198:GLY:H	2.25	0.49
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:CD2	2:B:296:HIS:CE1	2.99	0.49
2:D:176:PRO:HA	2:D:179:HIS:CG	2.48	0.48
1:A:160:TPO:N	1:A:160:TPO:O3P	2.39	0.48
1:A:106:SER:OG	1:A:291:LYS:HA	2.13	0.48
1:C:41:THR:HB	1:C:42:GLU:H	1.55	0.48
1:C:153:GLY:O	1:C:155:PRO:C	2.52	0.48
1:A:71:HIS:CE1	2:B:300:LYS:HG3	2.48	0.48
1:C:125:HIS:O	1:C:126:ARG:HB2	2.14	0.48
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.95	0.48
1:A:97:THR:C	1:A:98:GLY:O	2.50	0.48
1:A:107:TYR:CZ	1:A:135:ILE:HD13	2.48	0.48
2:B:334:MET:HE1	4:B:2024:HOH:O	2.14	0.48
1:A:283:HIS:ND1	1:A:284:PRO:HD2	2.28	0.48
1:A:98:GLY:HA3	1:A:199:ARG:NH2	2.29	0.47
1:A:129:LYS:HG3	1:A:131:GLN:HG2	1.95	0.47
2:D:176:PRO:HA	2:D:179:HIS:ND1	2.28	0.47
1:A:290:THR:O	1:A:292:PRO:HD3	2.13	0.47
2:D:361:HIS:O	2:D:363:ALA:N	2.47	0.47
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.49	0.47
1:C:101:LEU:O	1:C:101:LEU:HG	2.14	0.47
1:A:39:THR:HG21	2:B:289:LYS:HZ3	1.77	0.47
2:B:278:PHE:HA	2:B:281:ILE:HG12	1.96	0.47
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.49	0.47
2:D:345:ASP:HA	2:D:346:PRO:HA	1.69	0.47
2:B:285:THR:HG23	3:E:31:ASN:ND2	2.30	0.47
1:C:203:PHE:HB3	1:C:211:GLN:NE2	2.30	0.47
1:A:249:SER:HA	4:A:2067:HOH:O	2.13	0.46
2:D:321:HIS:HE1	2:D:379:LYS:HD2	1.79	0.46
2:D:388:LYS:O	2:D:392:MET:N	2.48	0.46
2:B:376:LEU:HA	2:B:376:LEU:HD23	1.71	0.46
2:B:323:GLN:HA	2:B:324:PRO:HA	1.75	0.46
2:D:201:LYS:HD3	2:D:201:LYS:O	2.15	0.46
2:D:327:CYS:HG	2:D:419:HIS:CD2	2.33	0.46
1:A:227:TRP:CG	1:A:230:VAL:HG13	2.50	0.46
1:C:60:HIS:HB3	1:C:63:ILE:HD12	1.97	0.46
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.97	0.46
1:A:107:TYR:O	1:A:111:LEU:HG	2.16	0.46
2:B:296:HIS:CD2	2:B:300:LYS:HE2	2.51	0.46
1:A:106:SER:CB	1:A:290:THR:O	2.54	0.46
2:D:194:LYS:CE	2:D:195:PRO:HD2	2.46	0.46
2:B:417:LYS:HE3	2:B:418:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:VAL:O	2:D:219:VAL:HG23	2.15	0.46
2:D:372:TRP:CD1	2:D:377:ILE:HG12	2.51	0.46
1:C:222:PRO:HB3	1:C:269:TYR:CD2	2.51	0.46
1:C:227:TRP:HB3	1:C:230:VAL:HG13	1.98	0.45
2:D:216:ASP:OD2	2:D:408:SER:HB2	2.16	0.45
2:B:183:HIS:HB2	2:B:317:GLN:NE2	2.30	0.45
1:A:87:LEU:O	1:A:91:MET:HG3	2.16	0.45
1:C:55:LEU:HA	1:C:55:LEU:HD12	1.78	0.45
2:D:274:GLU:HG2	2:D:277:GLU:OE2	2.17	0.45
1:A:106:SER:CB	1:A:292:PRO:HD2	2.46	0.45
1:C:39:THR:O	1:C:40:GLU:CD	2.55	0.45
2:D:313:GLN:O	2:D:316:THR:CG2	2.63	0.45
2:B:199:TYR:CD1	2:B:199:TYR:C	2.90	0.44
1:A:202:LEU:HD23	1:A:203:PHE:CE2	2.52	0.44
2:D:200:MET:HG2	2:D:208:ASN:OD1	2.16	0.44
1:A:39:THR:CG2	2:B:289:LYS:NZ	2.75	0.44
2:D:248:VAL:HG12	2:D:249:LEU:O	2.17	0.44
1:C:255:LEU:HD12	1:C:255:LEU:HA	1.78	0.44
2:D:388:LYS:HE3	2:D:432:LEU:HB3	1.98	0.44
1:A:148:LEU:HA	1:A:148:LEU:HD13	1.89	0.44
2:D:365:TYR:O	2:D:365:TYR:CG	2.70	0.44
1:A:39:THR:C	1:A:41:THR:N	2.70	0.44
2:B:229:ASN:HD22	2:B:334:MET:CE	2.31	0.44
1:C:203:PHE:CB	1:C:211:GLN:HE22	2.31	0.44
2:B:364:LEU:HG	2:B:370:GLN:HB2	1.98	0.44
1:A:97:THR:O	1:A:98:GLY:O	2.35	0.44
2:B:316:THR:HG21	4:B:2003:HOH:O	2.18	0.44
2:D:401:ALA:N	2:D:402:PRO:CD	2.80	0.44
1:A:140:ALA:HA	1:A:291:LYS:HE3	2.00	0.44
1:C:115:LEU:HD21	1:C:185:ASP:HB3	1.99	0.44
1:A:36:ARG:HH11	1:A:36:ARG:HG2	1.82	0.44
2:D:361:HIS:O	2:D:364:LEU:N	2.51	0.43
1:A:223:ASP:H	1:A:226:VAL:CG1	2.30	0.43
1:C:195:GLU:O	1:C:199:ARG:N	2.47	0.43
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.99	0.43
2:D:392:MET:HE2	2:D:430:LEU:HD12	2.01	0.43
1:A:88:LYS:HD2	1:A:131:GLN:OE1	2.18	0.43
2:D:380:THR:HB	2:D:382:TYR:CD2	2.53	0.43
2:D:388:LYS:HB3	2:D:389:PRO:HD3	2.00	0.43
2:D:308:ALA:O	2:D:313:GLN:NE2	2.51	0.43
2:B:225:TYR:CE1	2:B:281:ILE:HG21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:HIS:O	1:C:163:VAL:HG12	2.17	0.43
1:A:86:ASP:C	1:A:86:ASP:OD1	2.56	0.43
1:C:217:ARG:HH11	1:C:217:ARG:HB3	1.83	0.43
1:A:181:SER:O	1:A:184:VAL:HG22	2.18	0.43
2:D:175:VAL:O	2:D:177:ASP:N	2.46	0.43
1:C:217:ARG:NH1	1:C:217:ARG:HB3	2.34	0.43
1:A:9:LYS:HE3	1:A:17:VAL:HG13	2.01	0.43
1:A:36:ARG:HG2	1:A:36:ARG:NH1	2.33	0.43
1:A:278:LYS:HD2	2:B:177:ASP:OD1	2.18	0.43
1:C:167:TRP:CD1	1:C:204:PRO:HA	2.54	0.43
2:D:338:GLU:HB3	2:D:409:ILE:HD13	2.00	0.43
2:D:388:LYS:N	2:D:389:PRO:CD	2.82	0.42
1:C:52:ILE:O	1:C:56:LYS:HG3	2.19	0.42
1:A:249:SER:HA	1:A:260:ARG:HD3	2.01	0.42
1:C:216:PHE:O	1:C:220:GLY:N	2.52	0.42
1:C:231:THR:HG22	1:C:236:TYR:CZ	2.54	0.42
1:A:288:ASP:OD1	1:A:288:ASP:N	2.49	0.42
1:A:154:VAL:HA	1:A:155:PRO:HA	1.89	0.42
1:C:126:ARG:CD	1:C:163:VAL:HG21	2.45	0.42
2:D:360:PHE:CE2	2:D:376:LEU:HD11	2.55	0.42
2:B:194:LYS:HA	2:B:195:PRO:HD3	1.92	0.42
2:D:354:VAL:O	2:D:355:ILE:C	2.57	0.42
2:D:202:LYS:HA	2:D:202:LYS:HD2	1.78	0.42
1:A:34:LYS:HG2	1:A:35:ILE:N	2.34	0.42
1:A:163:VAL:HG22	1:A:164:VAL:N	2.35	0.42
2:D:316:THR:HG23	2:D:317:GLN:N	2.35	0.42
2:D:323:GLN:HA	2:D:324:PRO:HA	1.74	0.42
1:C:62:ASN:HA	1:C:142:LYS:HG2	2.01	0.42
1:C:229:GLY:O	1:C:233:MET:HG3	2.20	0.42
1:C:252:VAL:CG1	1:C:255:LEU:HB2	2.49	0.42
1:A:97:THR:CG2	1:A:97:THR:O	2.65	0.42
1:C:262:LEU:CG	1:C:266:MET:HE2	2.49	0.42
2:D:346:PRO:HD2	2:D:347:TYR:CE2	2.54	0.41
1:A:266:MET:O	1:A:274:ARG:HD3	2.20	0.41
1:C:101:LEU:N	1:C:102:PRO:CD	2.83	0.41
2:B:332:LEU:HD23	2:B:363:ALA:HA	2.01	0.41
1:C:49:ILE:CG2	2:D:306:LEU:HD12	2.51	0.41
1:C:227:TRP:HB3	1:C:230:VAL:CG1	2.49	0.41
1:A:88:LYS:O	1:A:90:PHE:N	2.53	0.41
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.72	0.41
2:D:383:THR:O	2:D:386:SER:OG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:ASP:HA	2:B:346:PRO:HA	1.74	0.41
1:C:38:ASP:C	1:C:39:THR:HG1	2.18	0.41
2:D:309:PRO:HA	2:D:313:GLN:NE2	2.35	0.41
1:C:60:HIS:HD2	1:C:62:ASN:N	2.04	0.41
1:C:154:VAL:HA	1:C:155:PRO:HA	1.84	0.41
1:A:101:LEU:N	1:A:102:PRO:HD2	2.36	0.41
1:A:161:HIS:CD2	4:A:2009:HOH:O	2.63	0.41
2:D:175:VAL:O	2:D:179:HIS:CE1	2.74	0.41
2:B:388:LYS:O	2:B:392:MET:HG2	2.21	0.41
2:D:335:PHE:CE2	2:D:339:LEU:HD11	2.55	0.41
2:D:273:PRO:HB2	2:D:278:PHE:CE2	2.56	0.41
1:A:227:TRP:O	1:A:230:VAL:HG22	2.21	0.41
1:A:71:HIS:CE1	2:B:296:HIS:CD2	3.07	0.41
1:A:106:SER:O	1:A:110:GLN:HG3	2.20	0.41
1:C:155:PRO:HD2	2:D:316:THR:HG1	1.85	0.41
1:A:255:LEU:HG	1:A:259:GLY:HA3	2.03	0.41
2:D:332:LEU:HD13	2:D:421:VAL:HB	2.03	0.41
1:A:126:ARG:HD2	1:A:163:VAL:HG21	2.03	0.41
1:A:222:PRO:HA	1:A:226:VAL:HG11	2.02	0.41
1:C:176:GLY:O	1:C:234:PRO:HG2	2.22	0.41
2:B:289:LYS:HE2	2:B:293:ARG:HH21	1.87	0.40
1:C:270:ASP:OD1	1:C:272:ASN:N	2.54	0.40
1:C:278:LYS:HE2	2:D:178:TYR:CE1	2.56	0.40
2:D:311:VAL:HG13	2:D:356:ALA:HB2	2.02	0.40
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.55	0.40
2:B:194:LYS:HD2	2:B:351:LEU:HD21	2.03	0.40
2:D:272:PRO:HA	2:D:273:PRO:HD3	2.00	0.40
1:A:217:ARG:HG2	1:A:243:TRP:CD2	2.56	0.40
2:D:308:ALA:HA	2:D:309:PRO:HD3	1.98	0.40
1:C:230:VAL:C	1:C:232:SER:H	2.24	0.40
2:D:372:TRP:HA	2:D:373:PRO:HD2	1.94	0.40
2:D:383:THR:O	2:D:386:SER:N	2.54	0.40
2:B:348:LEU:HD12	2:B:348:LEU:HA	1.90	0.40
1:C:284:PRO:HA	1:C:287:GLN:HE21	1.86	0.40
1:C:150:ARG:HH21	1:C:160:TPO:P	2.45	0.40
2:D:292:LEU:HA	2:D:292:LEU:HD12	1.88	0.40
2:D:359:ALA:HA	2:D:394:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.



## 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	295/303 (97%)	277 (94%)	14 (5%)	4 (1%)	14	10
1	C	288/303 (95%)	267 (93%)	16 (6%)	5 (2%)	11	7
2	B	256/259 (99%)	253 (99%)	3 (1%)	0	100	100
2	D	256/259 (99%)	236 (92%)	18 (7%)	2 (1%)	24	22
3	E	4/11 (36%)	3 (75%)	1 (25%)	0	100	100
All	All	1099/1135 (97%)	1036 (94%)	52 (5%)	11 (1%)	19	16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	197	VAL
1	A	98	GLY
1	A	164	VAL
1	C	84	HIS
1	C	162	GLU
1	C	220	GLY
1	C	38	ASP
1	A	41	THR
1	A	296	LEU
2	D	176	PRO
1	C	228	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/265 (98%)	250 (96%)	11 (4%)	36	44
1	C	256/265 (97%)	247 (96%)	9 (4%)	43	53
2	B	232/233 (100%)	224 (97%)	8 (3%)	44	54
2	D	232/233 (100%)	226 (97%)	6 (3%)	54	66
3	E	5/9 (56%)	5 (100%)	0	100	100
All	All	986/1005 (98%)	952 (97%)	34 (3%)	44	54

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	41	THR
1	A	55	LEU
1	A	74	ASN
1	A	75	LYS
1	A	89	LYS
1	A	122	ARG
1	A	131	GLN
1	A	150	ARG
1	A	248	PHE
1	A	255	LEU
2	B	179	HIS
2	B	232	LEU
2	B	296	HIS
2	B	316	THR
2	B	348	LEU
2	B	374	GLU
2	B	384	LEU
2	B	416	SER
1	C	39	THR
1	C	41	THR
1	C	55	LEU
1	C	75	LYS
1	C	88	LYS
1	C	122	ARG
1	C	131	GLN
1	C	148	LEU
1	C	150	ARG
2	D	177	ASP
2	D	232	LEU
2	D	245	SER

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Mol	Chain	Res	Type
2	D	292	LEU
2	D	304	PHE
2	D	348	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	85	GLN
1	A	119	HIS
2	B	179	HIS
2	B	229	ASN
2	B	233	HIS
2	B	254	GLN
2	B	431	ASN
1	C	60	HIS
1	C	71	HIS
1	C	84	HIS
1	C	119	HIS
1	C	121	HIS
1	C	268	HIS
1	C	287	GLN
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS
2	D	361	HIS
2	D	396	GLN
2	D	403	GLN
2	D	431	ASN

### 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	2.96	4 (50%)	7,14,16	2.22	2 (28%)
1	TPO	C	160	1	8,10,11	3.28	4 (50%)	7,14,16	2.93	4 (57%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-O3P	3.65	1.67	1.54
1	A	160	TPO	P-O3P	3.67	1.67	1.54
1	A	160	TPO	P-O1P	3.90	1.64	1.51
1	A	160	TPO	P-O2P	3.92	1.68	1.54
1	C	160	TPO	P-O2P	4.08	1.69	1.54
1	C	160	TPO	P-O1P	4.86	1.67	1.51
1	A	160	TPO	O-C	4.94	1.42	1.19
1	C	160	TPO	O-C	5.25	1.44	1.19

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O-C-CA	-4.94	112.38	125.44
1	A	160	TPO	O-C-CA	-4.51	113.52	125.44
1	C	160	TPO	C-CA-N	2.19	114.40	109.83
1	A	160	TPO	O2P-P-O1P	2.47	118.54	110.58
1	C	160	TPO	O3P-P-O2P	3.19	119.52	107.38
1	C	160	TPO	O2P-P-O1P	3.59	122.13	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	160	TPO	1	0
1	C	160	TPO	2	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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	296/303 (97%)	0.24	20 (6%) 20 20	20, 33, 82, 103	0
1	C	292/303 (96%)	0.58	41 (14%) 4 3	27, 47, 121, 150	0
2	B	258/259 (99%)	0.16	14 (5%) 29 29	21, 33, 55, 86	0
2	D	258/259 (99%)	0.75	37 (14%) 4 3	24, 52, 116, 146	0
3	E	6/11 (54%)	3.88	5 (83%) 0 0	142, 143, 148, 149	0
All	All	1110/1135 (97%)	0.45	117 (10%) 8 7	20, 40, 106, 150	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	ARG	8.6
1	A	96	LEU	8.5
1	A	97	THR	7.5
1	C	225	VAL	7.5
2	D	175	VAL	7.2
1	A	39	THR	6.9
1	C	15	TYR	6.9
2	D	432	LEU	6.8
3	E	35	PRO	6.8
1	C	233	MET	6.7
1	C	231	THR	6.3
1	C	226	VAL	6.2
1	C	249	SER	6.2
3	E	32	LEU	6.1
2	D	284	ASP	5.9
2	D	176	PRO	5.7
1	C	223	ASP	5.5
1	C	227	TRP	5.5
2	D	323	GLN	5.4
2	D	430	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	15	TYR	5.2
1	A	36	ARG	5.0
1	C	238	PRO	4.9
2	D	427	PRO	4.8
1	C	175	LEU	4.7
1	A	37	LEU	4.7
1	C	38	ASP	4.7
1	A	294	PRO	4.5
1	C	222	PRO	4.4
2	D	419	HIS	4.3
1	C	250	LYS	4.3
1	C	232	SER	4.2
1	C	244	ALA	3.9
2	B	176	PRO	3.9
3	E	33	PHE	3.8
1	C	14	THR	3.8
1	A	40	GLU	3.7
1	A	296	LEU	3.6
2	D	420	GLY	3.6
2	D	327	CYS	3.5
3	E	34	GLY	3.5
2	B	175	VAL	3.5
1	C	296	LEU	3.5
2	D	197	VAL	3.5
1	C	17	VAL	3.4
1	C	13	GLY	3.2
1	A	73	GLU	3.2
2	B	234	LEU	3.2
2	B	432	LEU	3.2
2	D	381	GLY	3.1
1	A	19	TYR	3.1
2	D	365	TYR	3.1
2	D	372	TRP	3.1
2	D	384	LEU	3.1
2	D	399	LEU	3.0
2	D	283	ASP	3.0
1	C	295	HIS	3.0
2	D	378	ARG	3.0
2	D	416	SER	2.9
1	C	12	GLU	2.9
2	B	341	LEU	2.9
2	D	428	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	253	PRO	2.9
1	A	95	ALA	2.9
1	A	14	THR	2.8
1	C	236	TYR	2.8
1	C	101	LEU	2.8
1	C	228	PRO	2.7
2	B	280	TYR	2.7
1	A	293	VAL	2.7
2	B	311	VAL	2.7
1	C	229	GLY	2.7
1	C	224	GLU	2.6
1	C	19	TYR	2.6
2	D	184	THR	2.6
2	D	370	GLN	2.6
1	C	161	HIS	2.5
1	C	230	VAL	2.5
2	B	323	GLN	2.5
2	D	280	TYR	2.5
2	D	232	LEU	2.5
2	B	431	ASN	2.4
2	D	373	PRO	2.4
2	D	392	MET	2.4
2	D	424	LEU	2.4
2	D	382	TYR	2.4
1	C	293	VAL	2.4
2	D	341	LEU	2.4
1	A	38	ASP	2.3
2	D	234	LEU	2.3
2	B	284	ASP	2.3
1	C	248	PHE	2.3
2	D	395	HIS	2.3
2	D	320	LEU	2.3
2	B	236	VAL	2.3
1	C	179	TYR	2.3
1	C	9	LYS	2.2
1	A	71	HIS	2.2
2	B	324	PRO	2.2
2	D	179	HIS	2.2
2	D	236	VAL	2.2
1	C	273	LYS	2.1
1	A	162	GLU	2.1
1	C	209	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	74	ASN	2.1
1	A	17	VAL	2.1
2	D	191	VAL	2.1
1	C	247	ASP	2.1
2	B	337	GLY	2.1
1	C	151	ALA	2.1
2	D	332	LEU	2.0
2	D	396	GLN	2.0
1	C	257	GLU	2.0
1	C	162	GLU	2.0
1	C	39	THR	2.0
2	B	310	THR	2.0
3	E	30	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	C	160	11/12	0.97	0.10	-	34,37,40,44	0
1	TPO	A	160	11/12	0.97	0.09	-	25,28,31,31	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.