



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2017 – 11:03 AM EST

PDB ID : 2WEV  
Title : Truncation and Optimisation of Peptide Inhibitors of CDK2, Cyclin A Through Structure Guided Design  
Authors : Kontopidis, G.; Andrews, M.J.; McInnes, C.; Plater, A.; Innes, L.; Renachowski, S.; Cowan, A.; Fischer, P.M.  
Deposited on : 2009-04-01  
Resolution : 2.30 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

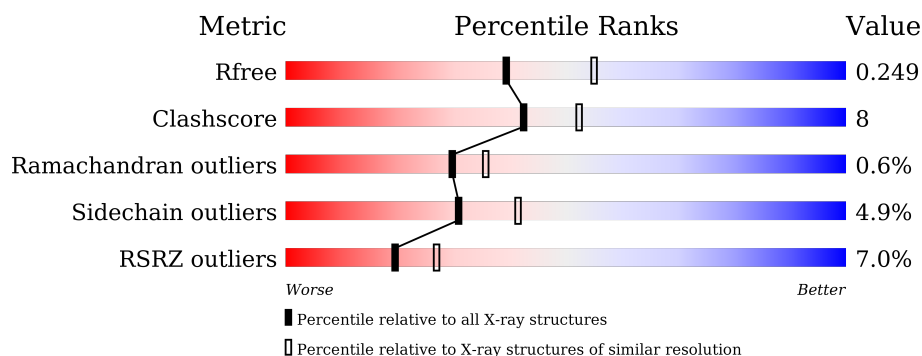
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	298	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>..</div> </div> </div>
1	C	298	<div> <div>10%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
2	B	260	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
2	D	260	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
3	E	6	<div> <div></div> <div> <div>50%</div> <div>33%</div> <div>17%</div> </div> </div>
3	F	6	<div> <div></div> <div> <div>33%</div> <div>50%</div> <div>17%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CK7	C	1298[B]	-	-	X	-
4	CK7	C	1298[C]	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9659 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	296	Total	C	N	O	S	0	0	0
			2377	1547	403	419	8			
1	C	297	Total	C	N	O	S	0	1	1
			2384	1550	404	422	8			

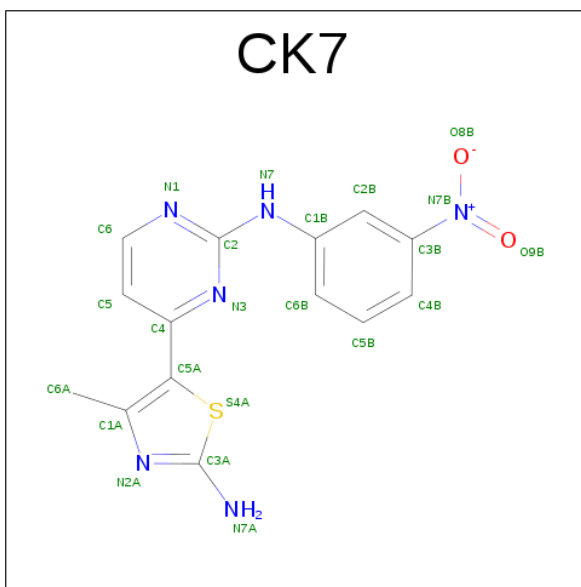
- Molecule 2 is a protein called CYCLIN-A2.

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
			2084	1350	339	384	11			

- Molecule 3 is a protein called ARG-ARG-B3L-MEA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	1
			47	31	11	5			
3	F	6	Total	C	N	O	0	0	1
			47	31	11	5			

- Molecule 4 is [4-(2-AMINO-4-METHYL-THIAZOL-5-YL)-PYRIMIDIN-2-YL]-(3-NITRO-PHENYL)-AMINE (three-letter code: CK7) (formula: C<sub>14</sub>H<sub>12</sub>N<sub>6</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			23	14	6	2	1		
4	C	1	Total	C	N	O	S	0	1
			69	42	18	6	3		

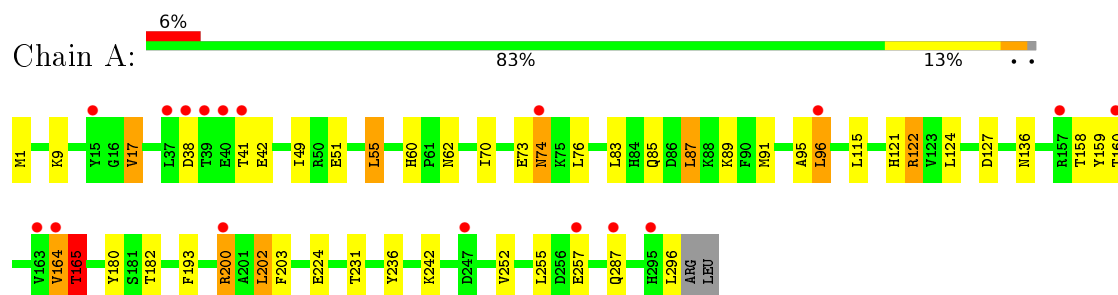
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	142	Total	O	0	0
			142	142		
5	B	127	Total	O	0	0
			127	127		
5	C	133	Total	O	0	0
			133	133		
5	D	143	Total	O	0	0
			143	143		

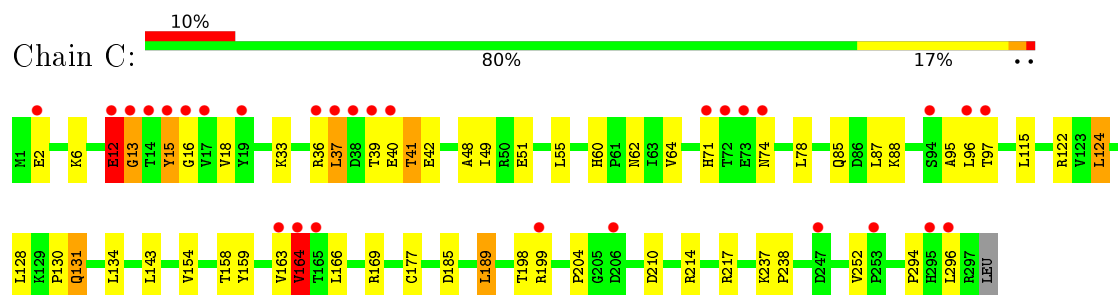
### 3 Residue-property plots

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

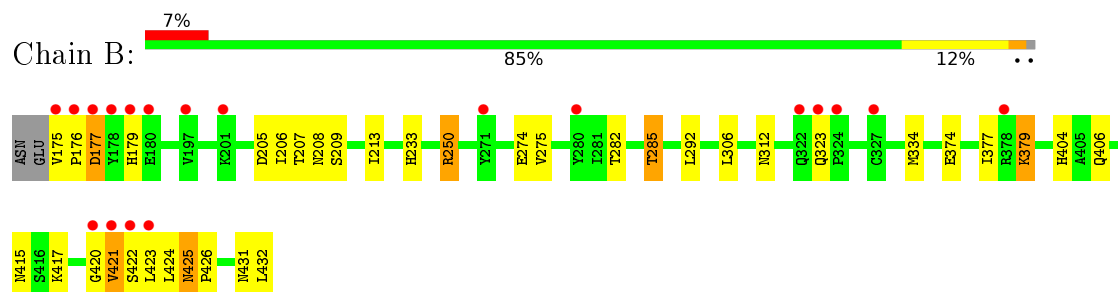
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



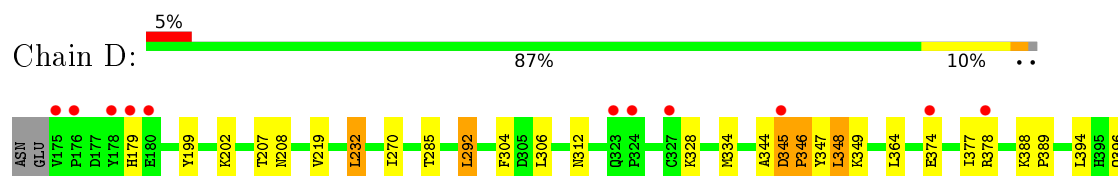
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



#### • Molecule 2: CYCLIN-A2



#### • Molecule 2: CYCLIN-A2





- Molecule 3: ARG-ARG-B3L-MEA



- Molecule 3: ARG-ARG-B3L-MEA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.52Å 113.84Å 158.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 12.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.00-2.30) 96.1 (12.00-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.85 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.187 , 0.243 0.193 , 0.249	Depositor DCC
$R_{free}$ test set	2911 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B3L, CK7, MEA, ACE, NH2

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	0.73	1/2439 (0.0%)	0.67	0/3312
1	C	0.71	0/2449	0.71	1/3326 (0.0%)
2	B	0.74	0/2133	0.66	0/2896
2	D	0.72	0/2134	0.62	0/2897
3	E	2.38	2/22 (9.1%)	1.70	0/27
3	F	2.26	2/22 (9.1%)	1.90	0/27
All	All	0.74	5/9199 (0.1%)	0.68	1/12485 (0.0%)

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	4
3	E	0	2
3	F	0	2
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	ARG	CD-NE	-7.58	1.33	1.46
3	E	3	ARG	CG-CD	-7.04	1.34	1.51
3	F	3	ARG	CG-CD	-7.00	1.34	1.51
3	F	3	ARG	CD-NE	-6.86	1.34	1.46
1	A	257	GLU	CG-CD	5.95	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	GLY	N-CA-C	-5.29	99.89	113.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	12	GLU	Peptide
1	C	163	VAL	Peptide
1	C	164	VAL	Peptide
1	C	37	LEU	Peptide
3	E	3	ARG	Sidechain,Peptide
3	F	3	ARG	Sidechain,Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2377	0	2426	38	0
1	C	2384	0	2430	64	1
2	B	2083	0	2107	24	1
2	D	2084	0	2107	21	0
3	E	47	0	52	3	0
3	F	47	0	52	4	0
4	A	23	0	12	3	0
4	C	69	0	36	24	0
5	A	142	0	0	7	0
5	B	127	0	0	2	0
5	C	133	0	0	2	0
5	D	143	0	0	2	0
All	All	9659	0	9222	153	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 8.

All (153) 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:C:33:LYS:NZ	4:C:1298[C]:CK7:H7A2	1.50	1.09
2:B:282:THR:O	2:B:285:THR:HG22	1.61	1.00
4:C:1298[A]:CK7:H5	4:C:1298[A]:CK7:H6A1	1.45	0.96
1:C:33:LYS:NZ	4:C:1298[C]:CK7:N7A	2.15	0.94
2:D:345:ASP:OD2	2:D:346:PRO:HD3	1.68	0.93
1:C:33:LYS:HZ2	4:C:1298[C]:CK7:H7A2	0.91	0.87
2:D:404:HIS:HD2	2:D:406:GLN:H	1.21	0.87
2:B:207:THR:HG22	2:B:209:SER:H	1.42	0.84
1:C:39:THR:HG22	1:C:41:THR:CG2	2.09	0.83
2:B:179:HIS:NE2	2:B:379:LYS:HE2	1.96	0.80
2:B:404:HIS:HD2	2:B:406:GLN:H	1.30	0.80
1:C:13:GLY:N	1:C:18:VAL:HG23	1.98	0.78
1:C:131:GLN:HE21	1:C:131:GLN:H	1.29	0.77
1:C:15:TYR:H	1:C:15:TYR:HD2	1.26	0.77
1:A:38:ASP:OD2	1:A:41:THR:HB	1.88	0.74
1:C:39:THR:HG22	1:C:41:THR:HG22	1.70	0.74
1:C:15:TYR:CD2	1:C:15:TYR:N	2.54	0.73
1:C:39:THR:HB	2:D:292:LEU:HD23	1.71	0.73
4:A:1297:CK7:H5	4:A:1297:CK7:H6A1	1.71	0.72
2:B:282:THR:O	2:B:285:THR:CG2	2.38	0.72
3:F:5:MEA:HC3	3:F:6:NH2:N	2.06	0.71
1:C:294:PRO:HG2	1:C:296:LEU:HD21	1.72	0.70
1:C:15:TYR:N	1:C:15:TYR:HD2	1.88	0.70
1:C:33:LYS:CE	4:C:1298[C]:CK7:H7A2	2.04	0.69
1:C:158:THR:HG21	1:C:177:CYS:O	1.91	0.69
1:C:33:LYS:CE	4:C:1298[C]:CK7:N7A	2.57	0.68
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.75	0.68
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.75	0.68
1:C:95:ALA:O	1:C:96:LEU:HG	1.95	0.67
1:C:51:GLU:O	1:C:55:LEU:HB2	1.96	0.66
1:C:39:THR:HA	1:C:41:THR:HG22	1.78	0.66
1:A:95:ALA:O	1:A:96:LEU:HB3	1.96	0.65
1:A:242:LYS:NZ	5:A:2108:HOH:O	2.29	0.65
1:C:159:TYR:CE1	2:D:270:ILE:HD12	2.32	0.65
1:C:60:HIS:CD2	1:C:62:ASN:H	2.15	0.65
4:A:1297:CK7:H2B	4:A:1297:CK7:N3	2.12	0.64
1:A:164:VAL:O	1:A:165:THR:HB	1.95	0.64
1:C:60:HIS:HD2	1:C:62:ASN:H	1.46	0.64
1:A:60:HIS:CD2	1:A:62:ASN:H	2.16	0.63
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.81	0.63
4:C:1298[A]:CK7:H6A2	5:C:2019:HOH:O	1.98	0.63
1:A:1:MET:HE3	1:A:70:ILE:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ALA:O	1:A:96:LEU:CB	2.48	0.62
1:C:33:LYS:HE3	4:C:1298[C]:CK7:N7A	2.15	0.62
4:C:1298[B]:CK7:H2B	4:C:1298[B]:CK7:H6A1	1.84	0.60
1:C:128:LEU:HD13	1:C:189:LEU:HD13	1.84	0.60
1:A:1:MET:CE	1:A:70:ILE:HD12	2.33	0.59
1:A:74:ASN:ND2	5:A:2046:HOH:O	2.36	0.58
1:A:193:PHE:CZ	1:A:255:LEU:HD21	2.38	0.58
1:A:60:HIS:HD2	1:A:62:ASN:H	1.50	0.58
2:D:207:THR:HG22	2:D:208:ASN:N	2.19	0.58
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.85	0.57
2:D:404:HIS:CD2	2:D:406:GLN:H	2.13	0.57
1:C:131:GLN:NE2	1:C:131:GLN:H	2.00	0.57
4:C:1298[A]:CK7:O8B	5:C:2133:HOH:O	2.17	0.57
1:C:198:THR:O	1:C:199:ARG:HB2	2.04	0.56
3:E:3:ARG:HH21	3:E:3:ARG:HB2	1.73	0.54
1:C:33:LYS:NZ	4:C:1298[B]:CK7:N7A	2.56	0.53
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.90	0.53
1:A:124:LEU:HD21	1:A:182:THR:HA	1.91	0.53
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.91	0.52
1:C:18:VAL:HG11	4:C:1298[B]:CK7:H6A2	1.90	0.52
1:C:40:GLU:O	1:C:41:THR:C	2.47	0.52
1:C:39:THR:CB	2:D:292:LEU:HD23	2.38	0.52
1:A:165:THR:O	1:A:165:THR:HG22	2.09	0.52
1:C:164:VAL:HG11	1:C:169:ARG:NH2	2.24	0.52
1:C:37:LEU:O	1:C:74:ASN:HB2	2.11	0.51
2:B:205:ASP:OD2	2:B:250:ARG:HD2	2.11	0.51
2:B:233:HIS:HD2	5:B:2071:HOH:O	1.94	0.51
2:B:420:GLY:O	2:B:421:VAL:C	2.49	0.51
1:C:85:GLN:HA	4:C:1298[C]:CK7:C5B	2.41	0.51
1:C:115:LEU:HD12	1:C:189:LEU:HD22	1.92	0.50
1:A:85:GLN:HE21	1:A:296:LEU:HD22	1.76	0.50
2:D:202:LYS:NZ	5:D:2031:HOH:O	2.43	0.50
1:A:158:THR:HA	1:A:180:TYR:CE1	2.47	0.50
1:C:64:VAL:HG22	1:C:143:LEU:O	2.13	0.49
4:C:1298[A]:CK7:H6A1	4:C:1298[A]:CK7:C5	2.28	0.49
2:B:404:HIS:CD2	2:B:406:GLN:H	2.20	0.49
1:C:78:LEU:N	1:C:78:LEU:HD23	2.26	0.49
1:A:85:GLN:NE2	1:A:296:LEU:HD22	2.28	0.48
1:A:51:GLU:O	1:A:55:LEU:HB2	2.14	0.48
2:D:349:LYS:NZ	5:D:2097:HOH:O	2.30	0.48
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1298[A]:CK7:H2B	4:C:1298[A]:CK7:N3	2.28	0.48
1:A:85:GLN:HG3	5:A:2053:HOH:O	2.12	0.48
2:B:207:THR:HG22	2:B:208:ASN:N	2.29	0.48
1:C:85:GLN:HA	4:C:1298[B]:CK7:C5B	2.43	0.48
4:C:1298[B]:CK7:N3	4:C:1298[B]:CK7:H6A1	2.29	0.47
4:C:1298[C]:CK7:H2B	4:C:1298[C]:CK7:N3	2.29	0.47
1:C:18:VAL:HG11	4:C:1298[B]:CK7:C6A	2.44	0.47
2:D:312:ASN:OD1	2:D:334:MET:CE	2.62	0.47
1:A:89:LYS:NZ	5:A:2053:HOH:O	2.47	0.47
2:B:420:GLY:O	2:B:422:SER:N	2.48	0.47
3:F:5:MEA:C1	3:F:6:NH2:N	2.74	0.47
1:C:71:HIS:NE2	2:D:304:PHE:HE2	2.13	0.47
3:E:4:B3L:HA	3:E:5:MEA:HC1	1.65	0.47
1:A:85:GLN:NE2	5:A:2051:HOH:O	2.47	0.46
1:A:42:GLU:OE2	2:B:275:VAL:HG23	2.14	0.46
1:A:17:VAL:HG12	5:A:2025:HOH:O	2.15	0.46
1:A:200:ARG:NE	5:A:2093:HOH:O	2.45	0.46
1:C:39:THR:CA	1:C:41:THR:HG22	2.45	0.46
4:C:1298[B]:CK7:H2B	4:C:1298[B]:CK7:N3	2.30	0.46
1:A:182:THR:HG1	2:B:175:VAL:N	2.13	0.46
1:A:1:MET:CE	1:A:70:ILE:CD1	2.94	0.46
1:C:71:HIS:CE1	2:D:304:PHE:HE2	2.33	0.45
4:C:1298[C]:CK7:H6A1	4:C:1298[C]:CK7:N3	2.31	0.45
2:B:175:VAL:HG13	2:B:177:ASP:HB2	1.98	0.45
4:A:1297:CK7:H6A1	4:A:1297:CK7:C5	2.45	0.45
1:C:252:VAL:HG23	1:C:252:VAL:O	2.17	0.45
1:C:39:THR:HA	1:C:40:GLU:C	2.37	0.45
1:C:12:GLU:C	1:C:18:VAL:HG23	2.36	0.45
1:A:159:TYR:N	1:A:159:TYR:HD1	2.15	0.45
1:C:164:VAL:HG21	1:C:166:LEU:HD21	1.98	0.45
2:B:312:ASN:OD1	2:B:334:MET:CE	2.65	0.45
1:C:96:LEU:HA	1:C:199:ARG:NH1	2.32	0.44
1:C:18:VAL:HG21	4:C:1298[B]:CK7:H6A2	2.00	0.44
2:B:420:GLY:O	2:B:423:LEU:N	2.34	0.44
2:D:347:TYR:OH	2:D:394:LEU:HA	2.18	0.44
2:D:388:LYS:HB3	2:D:389:PRO:HD3	2.00	0.43
1:A:127:ASP:OD1	1:A:164:VAL:O	2.35	0.43
1:C:39:THR:CG2	1:C:41:THR:HG22	2.45	0.43
1:A:159:TYR:N	1:A:159:TYR:CD1	2.85	0.43
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.00	0.43
1:A:121:HIS:O	1:A:122:ARG:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:HB	2:D:292:LEU:CD2	2.44	0.43
2:D:285:THR:HG23	3:F:3:ARG:NH1	2.34	0.43
1:A:73:GLU:OE2	1:C:2:GLU:HG2	2.18	0.43
1:A:231:THR:HG22	1:A:236:TYR:CZ	2.53	0.43
1:C:124:LEU:HD22	1:C:185:ASP:OD2	2.18	0.43
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.54	0.42
1:C:134:LEU:HD21	4:C:1298[C]:CK7:C6A	2.48	0.42
1:C:204:PRO:HD2	1:C:214:ARG:HD3	2.01	0.42
3:F:4:B3L:HA	3:F:5:MEA:HC1	1.67	0.42
2:B:175:VAL:O	2:B:177:ASP:N	2.53	0.42
2:B:213:ILE:HB	3:E:5:MEA:HE2	2.01	0.42
1:C:36:ARG:O	1:C:37:LEU:HD23	2.20	0.42
1:C:40:GLU:O	1:C:41:THR:O	2.38	0.42
1:A:87:LEU:O	1:A:91:MET:HG2	2.19	0.41
2:B:282:THR:HB	2:B:285:THR:HG23	2.01	0.41
1:C:40:GLU:O	2:D:292:LEU:HD21	2.19	0.41
1:C:95:ALA:O	1:C:96:LEU:CG	2.67	0.41
2:B:374:GLU:HA	2:B:377:ILE:HD12	2.02	0.41
1:A:1:MET:HE2	1:A:70:ILE:CD1	2.51	0.41
1:C:41:THR:HG23	1:C:42:GLU:N	2.36	0.41
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.91	0.41
2:B:425:ASN:HA	2:B:426:PRO:HD3	1.87	0.41
1:C:15:TYR:HE1	1:C:48:ALA:HB2	1.85	0.41
1:C:40:GLU:N	1:C:40:GLU:OE1	2.49	0.41
2:B:417:LYS:HG2	5:B:2122:HOH:O	2.19	0.41
1:C:237:LYS:HA	1:C:238:PRO:HD3	1.97	0.41
1:C:296:LEU:N	1:C:296:LEU:HD22	2.36	0.41
2:B:415:ASN:OD1	2:B:417:LYS:HB2	2.22	0.40
1:C:134:LEU:HD21	4:C:1298[C]:CK7:H6A3	2.03	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)
2:B:431:ASN:ND2	1:C:210[A]:ASP:OD1[2_664]	2.15	0.05

## 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	294/298 (99%)	288 (98%)	4 (1%)	2 (1%)	26	31
1	C	296/298 (99%)	285 (96%)	9 (3%)	2 (1%)	26	31
2	B	256/260 (98%)	249 (97%)	5 (2%)	2 (1%)	24	27
2	D	256/260 (98%)	253 (99%)	2 (1%)	1 (0%)	39	48
3	E	2/6 (33%)	2 (100%)	0	0	100	100
3	F	2/6 (33%)	2 (100%)	0	0	100	100
All	All	1106/1128 (98%)	1079 (98%)	20 (2%)	7 (1%)	30	36

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	THR
1	C	41	THR
1	A	96	LEU
2	B	176	PRO
2	B	421	VAL
1	C	16	GLY
2	D	346	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/263 (99%)	246 (94%)	15 (6%)	25	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	262/263 (100%)	250 (95%)	12 (5%)	33	44
2	B	232/234 (99%)	221 (95%)	11 (5%)	32	43
2	D	232/234 (99%)	221 (95%)	11 (5%)	32	43
3	E	2/2 (100%)	2 (100%)	0	100	100
3	F	2/2 (100%)	2 (100%)	0	100	100
All	All	991/998 (99%)	942 (95%)	49 (5%)	31	41

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	17	VAL
1	A	55	LEU
1	A	74	ASN
1	A	76	LEU
1	A	87	LEU
1	A	115	LEU
1	A	122	ARG
1	A	160	THR
1	A	164	VAL
1	A	165	THR
1	A	200	ARG
1	A	202	LEU
1	A	252	VAL
1	A	287	GLN
2	B	177	ASP
2	B	206	ILE
2	B	250	ARG
2	B	274	GLU
2	B	285	THR
2	B	292	LEU
2	B	323	GLN
2	B	379	LYS
2	B	424	LEU
2	B	425	ASN
2	B	432	LEU
1	C	6	LYS
1	C	12	GLU
1	C	15	TYR
1	C	87	LEU

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Mol	Chain	Res	Type
1	C	97	THR
1	C	122	ARG
1	C	124	LEU
1	C	131	GLN
1	C	154	VAL
1	C	164	VAL
1	C	189	LEU
1	C	217	ARG
2	D	179	HIS
2	D	199	TYR
2	D	232	LEU
2	D	292	LEU
2	D	328	LYS
2	D	345	ASP
2	D	348	LEU
2	D	364	LEU
2	D	378	ARG
2	D	396	GLN
2	D	424	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	74	ASN
1	A	85	GLN
1	A	268	HIS
1	A	295	HIS
2	B	208	ASN
2	B	233	HIS
2	B	296	HIS
2	B	323	GLN
2	B	404	HIS
2	B	419	HIS
2	B	431	ASN
1	C	60	HIS
1	C	131	GLN
1	C	287	GLN
2	D	208	ASN
2	D	233	HIS
2	D	296	HIS
2	D	322	GLN

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Mol	Chain	Res	Type
2	D	370	GLN
2	D	404	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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$
3	B3L	E	4	3	8,8,9	1.60	1 (12%)	8,9,11	1.62	1 (12%)
3	MEA	E	5	3	10,12,13	0.54	0	11,14,16	0.85	1 (9%)
3	B3L	F	4	3	8,8,9	1.83	1 (12%)	8,9,11	1.47	1 (12%)
3	MEA	F	5	3	10,12,13	0.70	0	11,14,16	0.79	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
3	B3L	E	4	3	-	0/7/7/8	0/0/0/0
3	MEA	E	5	3	-	0/4/8/10	0/1/1/1
3	B3L	F	4	3	-	0/7/7/8	0/0/0/0
3	MEA	F	5	3	-	0/4/8/10	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	B3L	CA-C	-4.83	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	B3L	CA-C	-4.14	1.36	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	MEA	C-CA-N	2.11	116.77	110.37
3	F	4	B3L	CB-CA-C	3.46	117.91	112.25
3	E	4	B3L	CB-CA-C	4.07	118.92	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	B3L	1	0
3	E	5	MEA	2	0
3	F	4	B3L	1	0
3	F	5	MEA	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z  > 2$
4	CK7	A	1297	-	19,25,25	0.84	1 (5%)	23,35,35	2.43	7 (30%)
4	CK7	C	1298[A]	-	19,25,25	0.69	0	23,35,35	3.20	8 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CK7	C	1298[B]	-	19,25,25	0.64	0	23,35,35	2.82	6 (26%)
4	CK7	C	1298[C]	-	19,25,25	0.61	0	23,35,35	2.79	7 (30%)

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
4	CK7	A	1297	-	-	0/8/12/12	0/3/3/3
4	CK7	C	1298[A]	-	-	2/8/12/12	0/3/3/3
4	CK7	C	1298[B]	-	-	0/8/12/12	0/3/3/3
4	CK7	C	1298[C]	-	-	0/8/12/12	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1297	CK7	C1B-N7	-2.52	1.35	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1298[A]	CK7	N1-C2-N3	-6.62	119.61	126.66
4	C	1298[B]	CK7	N1-C2-N3	-6.44	119.80	126.66
4	C	1298[C]	CK7	N1-C2-N3	-6.15	120.11	126.66
4	A	1297	CK7	N1-C2-N3	-4.92	121.42	126.66
4	C	1298[A]	CK7	C5-C6-N1	-4.09	119.08	123.88
4	C	1298[B]	CK7	C5-C6-N1	-3.42	119.88	123.88
4	C	1298[C]	CK7	C5-C6-N1	-3.23	120.10	123.88
4	A	1297	CK7	C5-C6-N1	-3.19	120.15	123.88
4	C	1298[A]	CK7	C5-C4-N3	-2.79	117.95	121.98
4	C	1298[C]	CK7	C5-C4-N3	-2.14	118.89	121.98
4	C	1298[A]	CK7	C3B-C2B-C1B	2.03	120.56	118.48
4	C	1298[C]	CK7	O9B-N7B-C3B	2.12	120.20	118.67
4	C	1298[A]	CK7	C6-C5-C4	2.16	119.26	117.28
4	A	1297	CK7	C3B-C2B-C1B	2.17	120.71	118.48
4	C	1298[B]	CK7	O9B-N7B-C3B	2.47	120.44	118.67
4	A	1297	CK7	O9B-N7B-C3B	2.53	120.49	118.67
4	A	1297	CK7	C5-C4-C5A	3.27	124.76	120.63
4	C	1298[A]	CK7	O9B-N7B-C3B	3.75	121.37	118.67
4	C	1298[B]	CK7	C5A-C4-N3	4.14	121.46	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1298[C]	CK7	C5A-C4-N3	4.43	121.80	116.58
4	A	1297	CK7	C6-N1-C2	5.53	119.70	115.42
4	C	1298[B]	CK7	C4-N3-C2	5.74	120.85	116.45
4	A	1297	CK7	C4-N3-C2	5.96	121.02	116.45
4	C	1298[C]	CK7	C4-N3-C2	6.39	121.36	116.45
4	C	1298[C]	CK7	C6-N1-C2	6.94	120.78	115.42
4	C	1298[A]	CK7	C4-N3-C2	7.44	122.16	116.45
4	C	1298[B]	CK7	C6-N1-C2	7.67	121.34	115.42
4	C	1298[A]	CK7	C6-N1-C2	8.38	121.90	115.42

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1298[A]	CK7	C4B-C3B-N7B-O9B
4	C	1298[A]	CK7	C2B-C3B-N7B-O9B

There are no ring outliers.

4 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1297	CK7	3	0
4	C	1298[A]	CK7	5	0
4	C	1298[B]	CK7	8	0
4	C	1298[C]	CK7	11	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	296/298 (99%)	0.10	17 (5%)	27 36	22, 32, 55, 72	1 (0%)
1	C	297/298 (99%)	0.44	29 (9%)	10 14	21, 33, 58, 75	1 (0%)
2	B	258/260 (99%)	0.22	19 (7%)	17 25	22, 35, 53, 74	0
2	D	258/260 (99%)	0.14	13 (5%)	32 41	23, 34, 52, 74	0
3	E	2/6 (33%)	0.44	0	100 100	35, 35, 35, 54	0
3	F	2/6 (33%)	0.09	0	100 100	40, 40, 40, 41	0
All	All	1113/1128 (98%)	0.23	78 (7%)	19 27	21, 34, 56, 75	2 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	THR	11.2
2	B	175	VAL	9.6
1	C	13	GLY	9.3
1	C	38	ASP	7.5
1	C	40	GLU	7.4
1	C	16	GLY	7.3
2	D	175	VAL	7.1
1	C	37	LEU	7.1
1	C	164	VAL	6.9
1	C	14	THR	6.3
2	B	271	TYR	6.3
2	B	324	PRO	6.0
1	C	12	GLU	5.6
2	B	323	GLN	5.2
1	C	71	HIS	5.1
1	C	36	ARG	5.1
2	D	432	LEU	4.9
1	C	15	TYR	4.8
2	B	178	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	72	THR	4.6
1	A	74	ASN	4.5
1	A	295	HIS	4.3
1	C	163	VAL	4.2
1	C	295	HIS	4.2
1	C	165	THR	4.0
2	B	422	SER	3.9
2	B	176	PRO	3.9
2	D	178	TYR	3.8
1	A	40	GLU	3.8
2	B	423	LEU	3.6
1	C	296	LEU	3.6
1	C	96	LEU	3.5
1	A	247	ASP	3.5
1	C	17	VAL	3.5
2	D	179	HIS	3.4
2	B	197	VAL	3.4
2	D	323	GLN	3.4
2	B	280	TYR	3.4
1	A	96	LEU	3.2
2	B	421	VAL	3.2
2	B	378	ARG	3.2
1	A	163	VAL	3.1
1	C	253	PRO	3.0
1	A	164	VAL	2.9
1	C	206	ASP	2.9
1	A	38	ASP	2.9
1	C	97	THR	2.8
1	C	74	ASN	2.8
2	D	327	CYS	2.8
2	D	378	ARG	2.8
1	A	15	TYR	2.8
2	B	180	GLU	2.7
2	D	176	PRO	2.7
1	A	41	THR	2.7
2	B	179	HIS	2.6
2	B	201	LYS	2.6
2	B	327	CYS	2.6
2	D	431	ASN	2.6
1	C	247	ASP	2.5
2	D	345	ASP	2.5
2	D	180	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLU	2.4
1	A	39	THR	2.4
1	C	73	GLU	2.3
1	A	157	ARG	2.3
2	D	324	PRO	2.3
1	A	200	ARG	2.3
1	C	94	SER	2.3
1	C	2	GLU	2.2
2	D	374	GLU	2.2
1	A	287	GLN	2.2
1	C	199	ARG	2.2
1	A	37	LEU	2.2
2	B	420	GLY	2.1
2	B	177	ASP	2.1
2	B	322	GLN	2.1
1	C	19	TYR	2.0
1	A	160	THR	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
3	B3L	F	4	9/10	0.95	0.10	-	29,30,32,33	0
3	MEA	E	5	12/13	0.76	0.21	-	34,36,48,55	0
3	MEA	F	5	12/13	0.86	0.18	-	31,35,41,43	0
3	B3L	E	4	9/10	0.85	0.22	-	28,32,37,39	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron



density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CK7	A	1297	23/23	0.92	0.14	0.11	25,30,52,57	0
4	CK7	C	1298[B]	23/23	0.92	0.17	-0.24	54,56,58,59	23
4	CK7	C	1298[A]	23/23	0.92	0.17	-0.28	15,29,42,45	23
4	CK7	C	1298[C]	23/23	0.92	0.17	-0.31	59,60,62,62	23

## 6.5 Other polymers

There are no such residues in this entry.