Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 10:57 pm GMT

PDB ID	:	2WFY
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	:	2009-04-15
Resolution	:	2.53 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

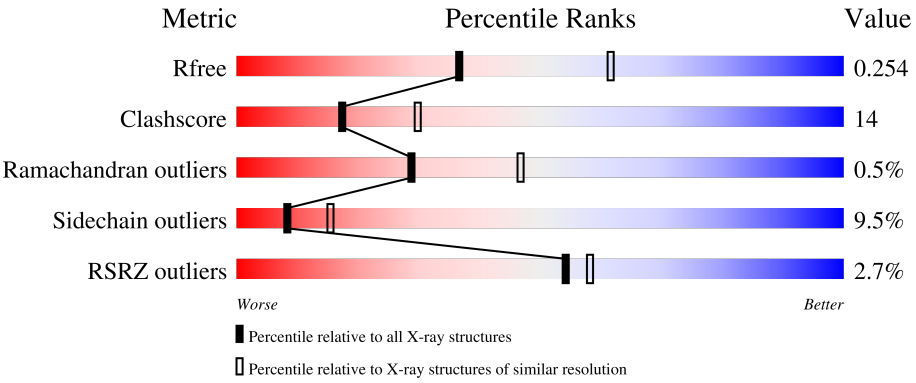
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	2% 72% 22% 5%
1	C	298	5% 69% 25% 5%
2	B	260	2% 78% 19%
2	D	260	2% 73% 25%
3	E	6	33% 17% 50%

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Mol	Chain	Length	Quality of chain
3	F	6	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9478 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	2	1
			2384	1550	406	420	8			
1	C	297	Total	C	N	O	S	0	0	1
			2379	1547	404	420	8			

- Molecule 2 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	1	0
			2081	1348	339	383	11			
2	D	260	Total	C	N	O	S	0	0	0
			2099	1359	342	387	11			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	1
			46	30	11	5			
3	F	6	Total	C	N	O	0	0	1
			46	30	11	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total	O	0	0
			126	126		
4	B	83	Total	O	0	0
			83	83		
4	C	125	Total	O	0	0
			125	125		
4	D	103	Total	O	0	0
			103	103		

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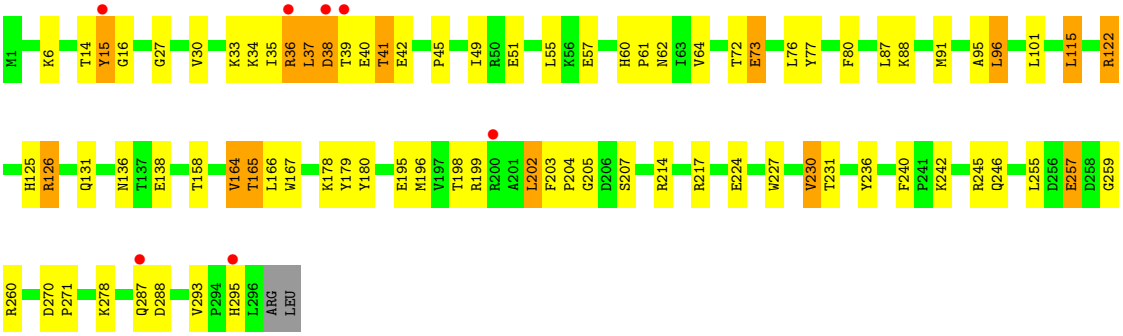
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	2	Total O 2 2	0	0
4	F	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

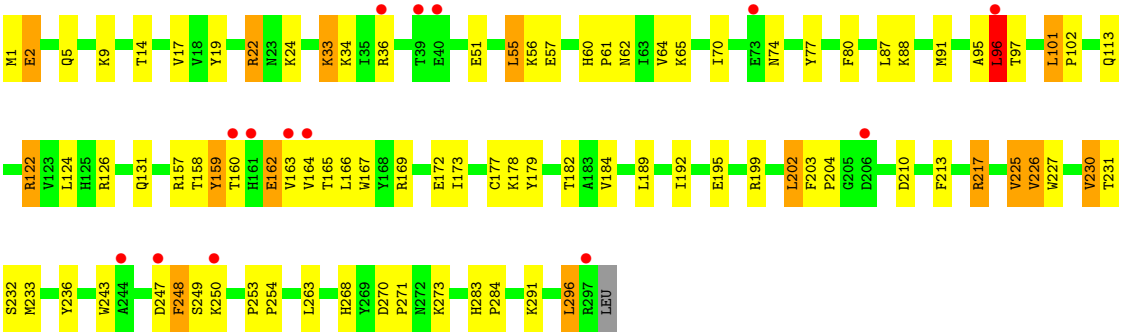
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A:



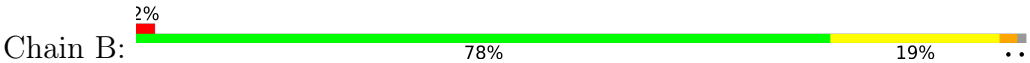
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

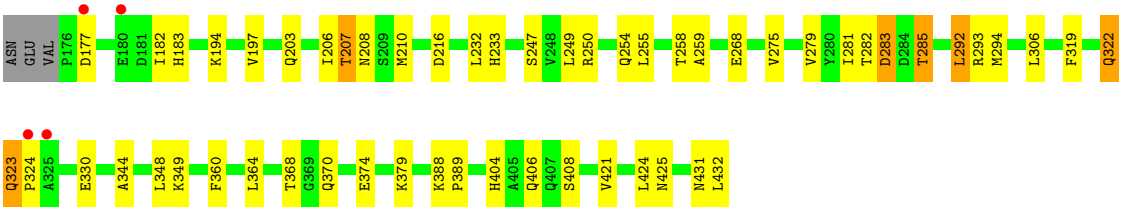
Chain C:



• Molecule 2: CYCLIN-A2

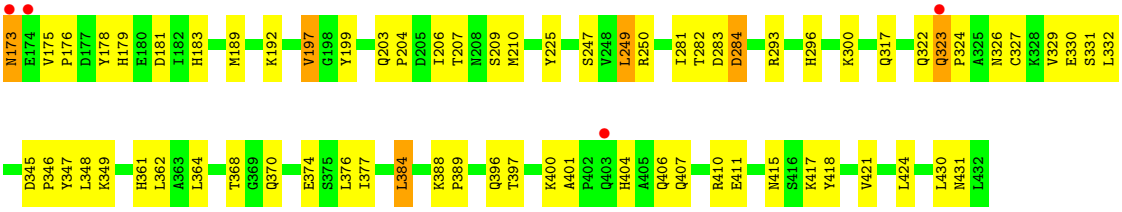
Chain B:





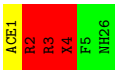
• Molecule 2: CYCLIN-A2

Chain D:



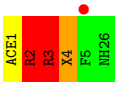
• Molecule 3: ARG-ARG-B3L-PHE

Chain E:



• Molecule 3: ARG-ARG-B3L-PHE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.62Å 115.81Å 157.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.53 12.20 – 2.53	Depositor EDS
% Data completeness (in resolution range)	92.2 (40.00-2.53) 93.1 (12.20-2.53)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.259 0.192 , 0.254	Depositor DCC
R_{free} test set	880 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9478	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NH2, ACE, B3L

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	0.65	0/2453	0.82	1/3331 (0.0%)
1	C	0.64	0/2441	0.80	1/3315 (0.0%)
2	B	0.59	0/2134	0.74	0/2898
2	D	0.65	1/2149 (0.0%)	0.76	0/2919
3	E	1.87	2/33 (6.1%)	1.72	0/40
3	F	1.98	2/33 (6.1%)	1.90	0/40
All	All	0.65	5/9243 (0.1%)	0.80	2/12543 (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
3	E	0	3
3	F	0	4
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	173	ASN	C-N	12.49	1.62	1.34
3	F	3	ARG	CB-CG	-7.48	1.32	1.52
3	F	2	ARG	CB-CG	-7.12	1.33	1.52
3	E	3	ARG	CB-CG	-6.98	1.33	1.52
3	E	2	ARG	CB-CG	-6.86	1.34	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	296	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	126	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	2	ARG	Sidechain
3	E	3	ARG	Sidechain
3	E	4	B3L	Peptide
3	F	2	ARG	Sidechain
3	F	3	ARG	Sidechain
3	F	4	B3L	Peptide,Mainchain

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	2384	0	2430	80	0
1	C	2379	0	2426	80	0
2	B	2081	0	2105	47	0
2	D	2099	0	2119	51	0
3	E	46	0	47	4	0
3	F	46	0	47	1	0
4	A	126	0	0	11	0
4	B	83	0	0	7	0
4	C	125	0	0	8	0
4	D	103	0	0	2	0
4	E	2	0	0	0	0
4	F	4	0	0	0	0
All	All	9478	0	9174	252	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 14.

All (252) 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:38:ASP:OD2	1:A:41:THR:HB	1.42	1.20
1:C:22:ARG:HG3	1:C:22:ARG:HH11	0.97	1.08
2:D:332:LEU:HB2	2:D:421:VAL:HG11	1.38	1.05
1:A:41:THR:HG22	1:A:42:GLU:H	1.22	1.03
1:C:95:ALA:O	1:C:96:LEU:HB3	1.57	1.01
2:D:207:THR:HG22	2:D:209:SER:H	1.26	1.01
2:B:282:THR:O	2:B:285:THR:HG22	1.60	1.01
1:A:15:TYR:CE2	1:A:33:LYS:HD2	1.99	0.97
1:A:88:LYS:HD2	1:A:131:GLN:HG2	1.42	0.97
2:B:404:HIS:CD2	2:B:406:GLN:H	1.85	0.95
2:D:418:TYR:O	2:D:421:VAL:HG23	1.66	0.95
1:C:22:ARG:HG3	1:C:22:ARG:NH1	1.71	0.94
2:B:421:VAL:HA	2:B:424:LEU:HD13	1.48	0.93
1:C:1:MET:HE3	1:C:70:ILE:HD12	1.48	0.93
1:A:41:THR:HG22	1:A:42:GLU:N	1.83	0.92
2:B:282:THR:HB	2:B:285:THR:HG23	1.54	0.90
1:A:164:VAL:CG1	1:A:164:VAL:O	2.21	0.88
1:A:38:ASP:OD2	1:A:41:THR:CB	2.22	0.88
2:D:332:LEU:HB2	2:D:421:VAL:CG1	2.04	0.88
2:D:404:HIS:HD2	2:D:406:GLN:H	1.21	0.88
2:B:404:HIS:HD2	2:B:406:GLN:H	0.92	0.87
1:A:60:HIS:HD2	1:A:62:ASN:H	1.21	0.85
1:C:162:GLU:HB2	1:C:169:ARG:HH12	1.40	0.84
2:B:254:GLN:O	2:B:258:THR:HG22	1.78	0.83
1:C:22:ARG:HH11	1:C:22:ARG:CG	1.88	0.82
1:A:41:THR:CG2	1:A:42:GLU:N	2.41	0.82
1:A:57:GLU:OE1	1:A:122:ARG:NH2	2.14	0.81
2:D:332:LEU:CB	2:D:421:VAL:HG11	2.12	0.80
1:A:15:TYR:CE2	1:A:33:LYS:CD	2.66	0.79
1:C:1:MET:CE	1:C:70:ILE:HD12	2.13	0.79
2:D:203:GLN:OE1	2:D:247:SER:HA	1.81	0.79
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.65	0.78
2:D:207:THR:HG22	2:D:209:SER:N	1.99	0.78
1:A:227:TRP:HB3	1:A:230:VAL:HG22	1.66	0.77
2:B:282:THR:HB	2:B:285:THR:CG2	2.12	0.77
2:B:404:HIS:HD2	2:B:406:GLN:N	1.77	0.76
1:C:217:ARG:HG3	1:C:217:ARG:HH11	1.52	0.74
2:B:282:THR:O	2:B:285:THR:CG2	2.35	0.72
1:A:60:HIS:CD2	1:A:62:ASN:H	2.06	0.71
1:C:227:TRP:O	1:C:230:VAL:HG22	1.89	0.71
1:C:162:GLU:CB	1:C:169:ARG:HH12	2.03	0.71
2:D:225:TYR:HE1	2:D:281:ILE:HG21	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:ASN:N	4:D:2011:HOH:O	2.23	0.70
1:C:51:GLU:HG3	1:C:55:LEU:HD22	1.74	0.70
1:A:164:VAL:O	1:A:164:VAL:HG13	1.91	0.69
2:D:415:ASN:OD1	2:D:417:LYS:HB3	1.92	0.69
1:C:217:ARG:HH11	1:C:217:ARG:CG	2.06	0.69
3:E:3:ARG:HG2	3:E:4:B3L:N	2.09	0.68
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.76	0.68
2:D:430:LEU:O	2:D:431:ASN:HB2	1.94	0.68
1:A:295:HIS:HB2	4:A:2126:HOH:O	1.94	0.67
1:C:124:LEU:HD21	1:C:182:THR:HA	1.75	0.67
1:A:73:GLU:HG2	1:C:2:GLU:HG2	1.76	0.67
1:A:198:THR:O	1:A:199:ARG:HB2	1.94	0.66
2:D:361:HIS:HE1	2:D:384:LEU:HD21	1.60	0.66
1:A:164:VAL:O	1:A:164:VAL:HG12	1.97	0.65
1:C:60:HIS:HD2	1:C:62:ASN:H	1.44	0.65
2:B:282:THR:O	2:B:283:ASP:HB2	1.97	0.65
1:C:159:TYR:HD1	1:C:159:TYR:N	1.94	0.65
2:B:374:GLU:HB3	4:B:2070:HOH:O	1.96	0.65
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.15	0.64
1:C:34:LYS:HE2	1:C:77:TYR:HE2	1.61	0.64
1:A:73:GLU:CG	1:C:2:GLU:HG2	2.27	0.64
1:C:217:ARG:HG3	1:C:217:ARG:NH1	2.08	0.64
2:D:404:HIS:CD2	2:D:406:GLN:H	2.09	0.64
1:C:213:PHE:O	1:C:217:ARG:HG2	1.97	0.64
1:A:57:GLU:CD	1:A:122:ARG:HH22	2.01	0.64
1:A:165:THR:HG23	1:A:165:THR:O	1.97	0.63
1:A:240:PHE:HB2	4:A:2106:HOH:O	1.98	0.63
1:A:42:GLU:OE2	2:B:275:VAL:HG23	1.99	0.62
1:A:41:THR:HG23	1:A:42:GLU:HG2	1.81	0.62
2:D:368:THR:OG1	2:D:370:GLN:HG3	1.99	0.61
1:C:51:GLU:O	1:C:55:LEU:HB2	2.00	0.61
1:C:60:HIS:CD2	1:C:62:ASN:H	2.17	0.61
2:B:203:GLN:OE1	2:B:247:SER:HA	2.01	0.61
1:C:159:TYR:N	1:C:159:TYR:CD1	2.67	0.61
1:C:91:MET:CE	1:C:195:GLU:HG2	2.31	0.61
1:C:166:LEU:HD23	1:C:169:ARG:HH21	1.65	0.60
1:C:172:GLU:HG2	1:C:271:PRO:HG3	1.82	0.60
1:C:9:LYS:CD	1:C:17:VAL:HG11	2.30	0.60
1:C:1:MET:HE2	1:C:1:MET:HA	1.84	0.60
1:C:162:GLU:HB2	1:C:169:ARG:NH1	2.15	0.60
2:B:183:HIS:HB2	4:B:2055:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:HD3	1:A:77:TYR:CE2	2.37	0.59
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.31	0.59
2:B:216:ASP:OD1	2:B:408:SER:HB2	2.03	0.59
2:B:364:LEU:HG	2:B:370:GLN:HB2	1.85	0.59
1:A:15:TYR:CD2	1:A:15:TYR:N	2.71	0.59
1:C:1:MET:CE	1:C:70:ILE:CD1	2.80	0.59
1:C:169:ARG:HB2	4:C:2071:HOH:O	2.03	0.58
2:D:332:LEU:HD13	2:D:421:VAL:HG12	1.84	0.58
2:D:418:TYR:O	2:D:421:VAL:CG2	2.48	0.58
2:D:176:PRO:HG2	2:D:179:HIS:HB2	1.86	0.58
2:B:207:THR:HG23	4:B:2019:HOH:O	2.04	0.57
2:B:233:HIS:HD2	4:B:2053:HOH:O	1.87	0.57
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.69	0.57
2:D:210:MET:CE	2:D:250:ARG:HB2	2.36	0.56
1:A:95:ALA:O	1:A:96:LEU:CB	2.53	0.56
2:D:361:HIS:CE1	2:D:384:LEU:HD21	2.39	0.56
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.87	0.56
1:A:51:GLU:O	1:A:55:LEU:HB2	2.06	0.56
1:A:95:ALA:O	1:A:96:LEU:HB3	2.06	0.56
1:A:73:GLU:OE1	2:B:293:ARG:NH2	2.38	0.56
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.36	0.56
2:D:332:LEU:CA	2:D:421:VAL:HG11	2.35	0.56
2:B:421:VAL:HA	2:B:424:LEU:CD1	2.31	0.55
1:A:16:GLY:HA2	4:A:2010:HOH:O	2.05	0.55
1:C:273:LYS:HE3	4:C:2109:HOH:O	2.07	0.55
1:A:125:HIS:O	1:A:126:ARG:HB2	2.07	0.55
1:C:225:VAL:HG12	1:C:226:VAL:N	2.22	0.55
1:A:15:TYR:HE2	1:A:33:LYS:CD	2.15	0.54
1:A:39:THR:HG21	4:A:2046:HOH:O	2.07	0.54
2:B:207:THR:HG22	2:B:208:ASN:H	1.72	0.54
2:D:361:HIS:HE1	2:D:384:LEU:CD2	2.21	0.54
1:C:159:TYR:HB2	1:C:162:GLU:HG2	1.89	0.53
1:C:231:THR:HG22	1:C:236:TYR:CE1	2.43	0.53
1:A:73:GLU:HG2	1:C:2:GLU:CG	2.38	0.53
2:B:322:GLN:HG3	2:B:360:PHE:HZ	1.73	0.53
1:C:9:LYS:HD2	1:C:17:VAL:HG11	1.89	0.53
1:A:227:TRP:HB3	1:A:230:VAL:CG2	2.36	0.53
1:A:49:ILE:CG2	2:B:306:LEU:HD12	2.38	0.53
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.91	0.53
1:A:33:LYS:HE2	1:A:80:PHE:CE1	2.44	0.53
2:D:210:MET:HE3	2:D:250:ARG:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:282:THR:O	2:D:283:ASP:CB	2.56	0.52
2:B:207:THR:H	2:B:210:MET:HG3	1.74	0.52
2:D:347:TYR:OH	2:D:397:THR:OG1	2.22	0.52
1:C:204:PRO:HD2	4:C:2090:HOH:O	2.10	0.52
1:C:91:MET:HE3	1:C:195:GLU:HG2	1.91	0.52
1:C:5:GLN:HB2	1:C:24:LYS:HD3	1.91	0.51
1:C:101:LEU:HB2	4:C:2048:HOH:O	2.10	0.51
1:C:247:ASP:HB2	1:C:250:LYS:HE2	1.92	0.51
2:D:347:TYR:HH	2:D:397:THR:HG1	1.56	0.51
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.93	0.51
1:C:33:LYS:HD3	1:C:80:PHE:CE1	2.46	0.51
3:E:2:ARG:HD2	3:E:4:B3L:H2E1	1.93	0.51
2:B:203:GLN:CG	2:B:206:ILE:HG12	2.41	0.50
2:D:322:GLN:NE2	2:D:326:ASN:H	2.09	0.50
1:A:27:GLY:HA3	2:D:249:LEU:HD22	1.92	0.50
1:C:124:LEU:CD2	1:C:182:THR:HA	2.42	0.50
1:A:38:ASP:HB3	4:A:2032:HOH:O	2.12	0.50
1:C:1:MET:HE3	1:C:70:ILE:CD1	2.31	0.50
1:C:19:TYR:HD1	4:C:2021:HOH:O	1.93	0.50
1:A:131:GLN:HG3	4:A:2063:HOH:O	2.11	0.49
1:A:158:THR:HA	1:A:180:TYR:CE1	2.47	0.49
1:A:278:LYS:HB3	4:B:2010:HOH:O	2.11	0.49
2:B:203:GLN:HG2	2:B:206:ILE:HG12	1.94	0.49
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.48	0.49
1:A:15:TYR:OH	1:A:51:GLU:OE1	2.28	0.49
1:C:247:ASP:HB2	1:C:250:LYS:CE	2.43	0.49
1:A:36:ARG:H	1:A:36:ARG:HG2	1.30	0.49
1:A:227:TRP:O	1:A:230:VAL:HG22	2.12	0.49
1:A:231:THR:HG22	1:A:236:TYR:CZ	2.48	0.49
2:D:203:GLN:HG2	2:D:206:ILE:CG1	2.44	0.48
2:D:407:GLN:O	2:D:411:GLU:HG2	2.13	0.48
1:A:164:VAL:O	1:A:165:THR:O	2.31	0.48
1:C:217:ARG:HD3	1:C:243:TRP:CZ3	2.49	0.47
1:A:165:THR:O	1:A:165:THR:CG2	2.62	0.47
2:B:388:LYS:HG3	2:B:432:LEU:HD13	1.95	0.47
2:D:331:SER:CB	2:D:421:VAL:HG21	2.44	0.47
2:B:344:ALA:O	2:B:348:LEU:HB2	2.14	0.47
1:C:169:ARG:HD2	1:C:173:ILE:HG21	1.96	0.47
3:E:2:ARG:HD2	3:E:4:B3L:CE1	2.44	0.47
1:A:288:ASP:OD1	1:A:288:ASP:N	2.48	0.47
1:C:169:ARG:HD2	1:C:173:ILE:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LYS:HD3	1:C:179:TYR:CE2	2.50	0.47
1:C:268:HIS:CE1	4:C:2091:HOH:O	2.67	0.47
1:A:198:THR:O	1:A:199:ARG:CB	2.63	0.47
2:B:319:PHE:CD2	2:B:330:GLU:HG2	2.50	0.47
2:B:255:LEU:HA	2:B:258:THR:CG2	2.45	0.47
1:A:204:PRO:HG2	1:A:214:ARG:NH1	2.29	0.47
2:B:292:LEU:HD12	2:B:292:LEU:HA	1.68	0.46
1:C:57:GLU:OE1	1:C:122:ARG:NH2	2.48	0.46
1:C:9:LYS:HD3	1:C:17:VAL:HG11	1.97	0.46
2:D:178:TYR:O	2:D:181:ASP:HB2	2.15	0.46
1:A:72:THR:HB	4:A:2045:HOH:O	2.15	0.46
2:B:421:VAL:CA	2:B:424:LEU:HD13	2.34	0.46
2:B:324:PRO:HA	4:B:2057:HOH:O	2.16	0.46
2:B:283:ASP:OD2	3:E:1:ACE:H1	2.17	0.45
2:D:203:GLN:HA	2:D:204:PRO:HD3	1.80	0.45
1:C:227:TRP:CD2	1:C:230:VAL:HG13	2.52	0.45
1:A:15:TYR:CZ	1:A:33:LYS:HD2	2.49	0.45
1:C:22:ARG:NH1	1:C:22:ARG:CG	2.55	0.45
2:D:430:LEU:O	2:D:431:ASN:CB	2.64	0.45
1:C:91:MET:HE1	1:C:195:GLU:HG2	1.98	0.45
1:A:231:THR:HA	1:A:236:TYR:CD1	2.51	0.45
1:C:97:THR:HA	4:C:2047:HOH:O	2.16	0.45
2:D:327:CYS:HA	2:D:330:GLU:HG3	1.98	0.45
1:A:40:GLU:HG3	4:A:2033:HOH:O	2.16	0.45
2:D:384:LEU:HD12	2:D:384:LEU:O	2.16	0.45
2:D:300:LYS:HB3	2:D:300:LYS:HE2	1.77	0.45
2:B:275:VAL:O	2:B:279:VAL:HG23	2.17	0.44
2:D:361:HIS:CE1	2:D:384:LEU:CD2	3.00	0.44
2:B:255:LEU:HA	2:B:258:THR:HG22	1.99	0.44
1:A:60:HIS:HD2	1:A:62:ASN:N	2.01	0.44
2:B:323:GLN:HG2	2:B:323:GLN:O	2.17	0.44
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.78	0.44
2:B:203:GLN:HG2	2:B:206:ILE:CG1	2.48	0.44
1:C:96:LEU:HG	1:C:97:THR:HG23	1.99	0.44
1:A:36:ARG:HG2	4:A:2014:HOH:O	2.18	0.44
1:A:91:MET:HE3	1:A:196:MET:HA	2.00	0.44
1:C:163:VAL:O	1:C:163:VAL:HG22	2.18	0.44
2:B:268:GLU:HG3	2:B:268:GLU:O	2.18	0.43
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.87	0.43
1:A:202:LEU:HD13	1:A:203:PHE:CZ	2.52	0.43
1:A:122:ARG:HB3	2:B:182:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD23	1:A:205:GLY:O	2.17	0.43
2:D:331:SER:HB3	2:D:421:VAL:HG21	1.99	0.43
2:D:346:PRO:O	2:D:349:LYS:HG2	2.18	0.43
1:C:270:ASP:OD1	1:C:271:PRO:HD2	2.18	0.43
2:D:329:VAL:HG11	2:D:364:LEU:HD13	2.01	0.43
1:C:164:VAL:HG23	4:C:2071:HOH:O	2.19	0.43
1:C:189:LEU:HD12	1:C:189:LEU:HA	1.92	0.43
2:D:225:TYR:CE1	2:D:281:ILE:HG21	2.45	0.43
2:B:259:ALA:CB	2:B:294:MET:HG3	2.49	0.42
4:D:2031:HOH:O	3:F:1:ACE:H2	2.19	0.42
1:A:178:LYS:HD3	1:A:179:TYR:CZ	2.54	0.42
2:B:368:THR:OG1	2:B:370:GLN:CG	2.68	0.42
1:A:37:LEU:HA	1:A:37:LEU:HD12	1.82	0.42
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.54	0.42
1:A:270:ASP:HA	1:A:271:PRO:HD3	1.91	0.42
1:A:73:GLU:HG2	1:C:2:GLU:CD	2.40	0.42
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.55	0.42
1:C:34:LYS:HE2	1:C:77:TYR:CE2	2.48	0.42
1:C:96:LEU:H	1:C:199:ARG:HH11	1.67	0.42
1:A:136:ASN:OD1	1:A:138:GLU:N	2.46	0.41
2:B:210:MET:HG2	4:B:2022:HOH:O	2.21	0.41
1:C:189:LEU:HD12	1:C:192:ILE:HD12	2.02	0.41
1:A:45:PRO:O	1:A:49:ILE:HG12	2.21	0.41
1:A:131:GLN:CG	4:A:2063:HOH:O	2.68	0.41
2:D:189:MET:SD	2:D:192:LYS:HD2	2.60	0.41
2:D:323:GLN:HA	2:D:324:PRO:HA	1.87	0.41
2:D:388:LYS:HB3	2:D:389:PRO:CD	2.48	0.41
1:C:177:CYS:HB3	1:C:233:MET:HE1	2.02	0.41
1:C:248:PHE:HE2	1:C:263:LEU:HD23	1.86	0.41
1:A:167:TRP:CE2	1:A:204:PRO:HA	2.55	0.41
1:A:91:MET:HE2	1:A:195:GLU:HG2	2.02	0.41
2:D:282:THR:O	2:D:283:ASP:HB2	2.20	0.41
2:B:282:THR:C	2:B:285:THR:HG22	2.35	0.41
1:C:126:ARG:HH11	1:C:126:ARG:HG2	1.86	0.41
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.56	0.40
1:C:173:ILE:HD11	1:C:184:VAL:HG11	2.03	0.40
2:D:400:LYS:O	2:D:401:ALA:C	2.59	0.40
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.56	0.40
1:A:257:GLU:OE1	1:A:260:ARG:NH2	2.54	0.40
1:C:101:LEU:N	1:C:102:PRO:CD	2.84	0.40
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:LYS:HB3	2:B:389:PRO:HD3	2.03	0.40
2:D:376:LEU:HD23	2:D:376:LEU:HA	1.77	0.40
1:A:217:ARG:NH1	4:A:2101:HOH:O	2.54	0.40
1:C:167:TRP:N	1:C:167:TRP:CD1	2.89	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	296/298 (99%)	281 (95%)	13 (4%)	2 (1%)	22 37
1	C	295/298 (99%)	279 (95%)	15 (5%)	1 (0%)	41 59
2	B	256/260 (98%)	246 (96%)	10 (4%)	0	100 100
2	D	258/260 (99%)	248 (96%)	8 (3%)	2 (1%)	19 33
3	E	3/6 (50%)	1 (33%)	1 (33%)	1 (33%)	0 0
3	F	3/6 (50%)	2 (67%)	1 (33%)	0	100 100
All	All	1111/1128 (98%)	1057 (95%)	48 (4%)	6 (0%)	29 47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	165	THR
1	C	96	LEU
2	D	284	ASP
2	D	197	VAL
3	E	2	ARG

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	262/263 (100%)	235 (90%)	27 (10%)	7 13
1	C	261/263 (99%)	227 (87%)	34 (13%)	4 7
2	B	232/234 (99%)	216 (93%)	16 (7%)	15 28
2	D	234/234 (100%)	219 (94%)	15 (6%)	17 31
3	E	3/3 (100%)	2 (67%)	1 (33%)	0 0
3	F	3/3 (100%)	1 (33%)	2 (67%)	0 0
All	All	995/1000 (100%)	900 (90%)	95 (10%)	8 15

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	14	THR
1	A	15	TYR
1	A	30	VAL
1	A	35	ILE
1	A	36	ARG
1	A	37	LEU
1	A	38	ASP
1	A	41	THR
1	A	64	VAL
1	A	73	GLU
1	A	76	LEU
1	A	87	LEU
1	A	101	LEU
1	A	115	LEU
1	A	122	ARG
1	A	164	VAL
1	A	202	LEU
1	A	207	SER
1	A	230	VAL
1	A	242	LYS
1	A	245	ARG

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Mol	Chain	Res	Type
1	A	246	GLN
1	A	257	GLU
1	A	287[A]	GLN
1	A	287[B]	GLN
1	A	293	VAL
2	B	177	ASP
2	B	194	LYS
2	B	197	VAL
2	B	207	THR
2	B	232	LEU
2	B	249	LEU
2	B	250	ARG
2	B	281	ILE
2	B	283	ASP
2	B	285	THR
2	B	292	LEU
2	B	322	GLN
2	B	323	GLN
2	B	349	LYS
2	B	379	LYS
2	B	431	ASN
1	C	2	GLU
1	C	14	THR
1	C	22	ARG
1	C	33	LYS
1	C	36	ARG
1	C	55	LEU
1	C	56	LYS
1	C	64	VAL
1	C	65	LYS
1	C	74	ASN
1	C	87	LEU
1	C	88	LYS
1	C	96	LEU
1	C	101	LEU
1	C	113	GLN
1	C	122	ARG
1	C	131	GLN
1	C	157	ARG
1	C	158	THR
1	C	159	TYR
1	C	160	THR

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Mol	Chain	Res	Type
1	C	162	GLU
1	C	165	THR
1	C	202	LEU
1	C	210	ASP
1	C	217	ARG
1	C	225	VAL
1	C	226	VAL
1	C	230	VAL
1	C	232	SER
1	C	248	PHE
1	C	249	SER
1	C	291	LYS
1	C	296	LEU
2	D	175	VAL
2	D	197	VAL
2	D	199	TYR
2	D	249	LEU
2	D	284	ASP
2	D	293	ARG
2	D	296	HIS
2	D	323	GLN
2	D	345	ASP
2	D	348	LEU
2	D	362	LEU
2	D	384	LEU
2	D	396	GLN
2	D	410	ARG
2	D	424	LEU
3	E	2	ARG
3	F	2	ARG
3	F	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	85	GLN
2	B	208	ASN
2	B	321	HIS
2	B	370	GLN
2	B	404	HIS
2	B	431	ASN

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Mol	Chain	Res	Type
1	C	60	HIS
1	C	71	HIS
1	C	85	GLN
1	C	287	GLN
2	D	179	HIS
2	D	208	ASN
2	D	229	ASN
2	D	317	GLN
2	D	322	GLN
2	D	361	HIS
2	D	396	GLN
2	D	404	HIS
2	D	431	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
3	B3L	F	4	3	8,8,9	1.72	1 (12%)	7,9,11	2.48	2 (28%)
3	B3L	E	4	3	8,8,9	1.78	1 (12%)	7,9,11	3.38	3 (42%)

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	F	4	3	-	1/7/7/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B3L	E	4	3	-	2/7/7/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	B3L	CB-C	-4.96	1.37	1.49
3	F	4	B3L	CB-C	-4.84	1.37	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	4	B3L	CA-CB-C	8.23	124.36	112.25
3	F	4	B3L	CA-CB-C	5.84	120.84	112.25
3	E	4	B3L	CD-CG-CA	2.55	125.86	116.39
3	E	4	B3L	O-C-CB	-2.21	118.97	125.43
3	F	4	B3L	O-C-CB	-2.14	119.19	125.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	4	B3L	N-CA-CG-CD
3	F	4	B3L	N-CA-CG-CD
3	E	4	B3L	N-CA-CB-C

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	B3L	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	173:ASN	C	174:GLU	N	1.62

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^{th} 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^2)	Q<0.9
1	A	296/298 (99%)	-0.27	7 (2%) 59 62	34, 47, 74, 90	0
1	C	297/298 (99%)	-0.21	14 (4%) 31 34	33, 48, 74, 91	0
2	B	257/260 (98%)	-0.30	4 (1%) 72 74	34, 53, 73, 86	0
2	D	260/260 (100%)	-0.26	4 (1%) 73 76	31, 52, 72, 99	0
3	E	3/6 (50%)	0.31	0 100 100	56, 56, 59, 59	3 (100%)
3	F	3/6 (50%)	1.05	1 (33%) 0 0	53, 53, 57, 57	3 (100%)
All	All	1116/1128 (98%)	-0.25	30 (2%) 54 58	31, 50, 74, 99	6 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	THR	7.4
2	D	173	ASN	5.4
1	C	161	HIS	4.6
1	C	164	VAL	4.2
2	D	174	GLU	4.0
1	C	40	GLU	3.8
1	C	163	VAL	3.8
1	A	36	ARG	3.7
1	A	15	TYR	3.3
1	C	96	LEU	3.1
1	A	39	THR	3.0
2	B	177	ASP	2.8
1	A	287[A]	GLN	2.8
2	B	180	GLU	2.8
1	C	250	LYS	2.7
2	D	323	GLN	2.6
2	B	324	PRO	2.5
1	C	244	ALA	2.4
1	C	206	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	36	ARG	2.4
1	C	160	THR	2.3
1	A	295	HIS	2.2
1	A	200	ARG	2.2
2	B	325	ALA	2.2
3	F	5	PHE	2.2
1	C	247	ASP	2.1
1	C	73	GLU	2.1
1	A	38	ASP	2.1
2	D	403	GLN	2.1
1	C	297	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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
3	B3L	F	4	9/10	0.89	0.18	45,52,56,59	9
3	B3L	E	4	9/10	0.94	0.14	49,50,57,59	9

6.3 Carbohydrates (i)

There are no monosaccharides 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.