Full wwPDB X-ray Structure Validation Report (i)

Dec 9, 2023 – 12:55 pm GMT

PDB ID	:	2WMA
Title	:	Structural and thermodynamic consequences of cyclization of peptide ligands for the recruitment site of cyclin A
Authors	:	Robertson, G.F.; Endicott, J.A.; Noble, M.E.M.; McDonnell, J.M.
Deposited on	:	2009-06-30
Resolution	:	2.80 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:

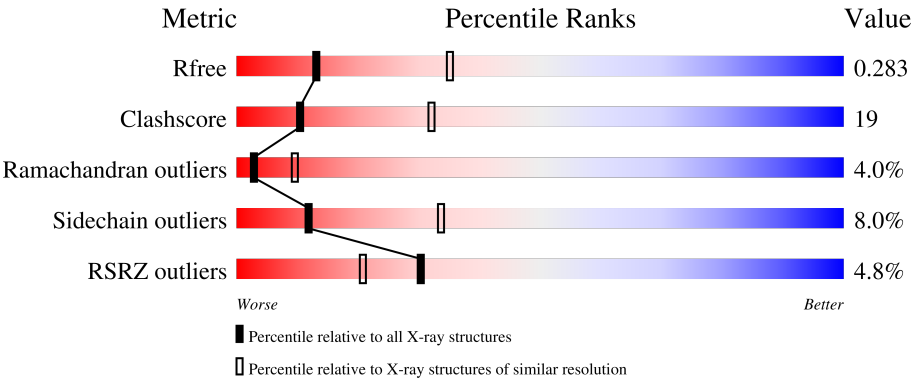
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	303	3% 61% 30% 7% ·
1	C	303	6% 50% 26% 11% · 12%
2	B	259	3% 68% 27% ·
2	D	259	7% 65% 30% ·
3	E	5	20% 40% 60%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8827 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	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			
1	C	266	Total	C	N	O	P	S	0	0	0
			2131	1380	364	379	1	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P24941
A	-3	PRO	-	expression tag	UNP P24941
A	-2	LEU	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-4	GLY	-	expression tag	UNP P24941
C	-3	PRO	-	expression tag	UNP P24941
C	-2	LEU	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is a protein called CYCLIC RKLFN-NH2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			47	31	10	6			

- Molecule 4 is water.

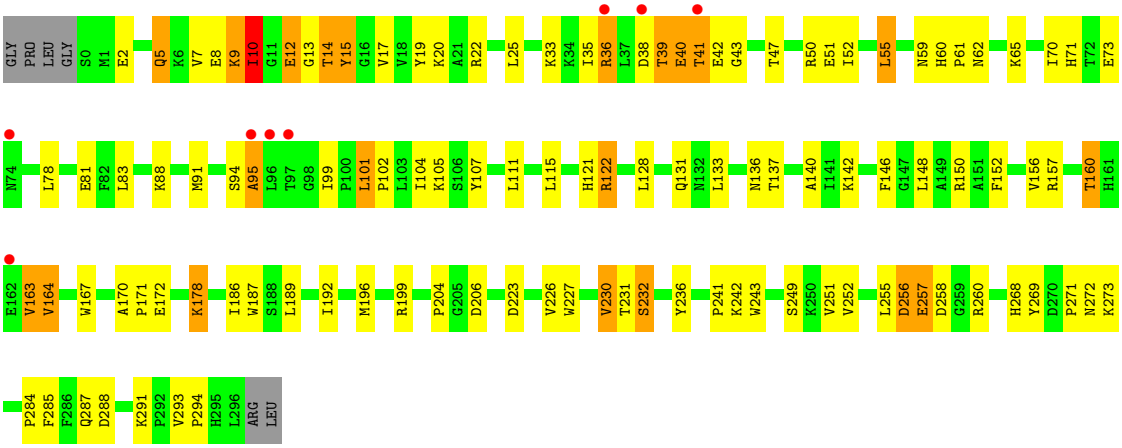
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	32	Total O 32 32	0	0
4	C	15	Total O 15 15	0	0
4	D	16	Total O 16 16	0	0

3 Residue-property plots

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.

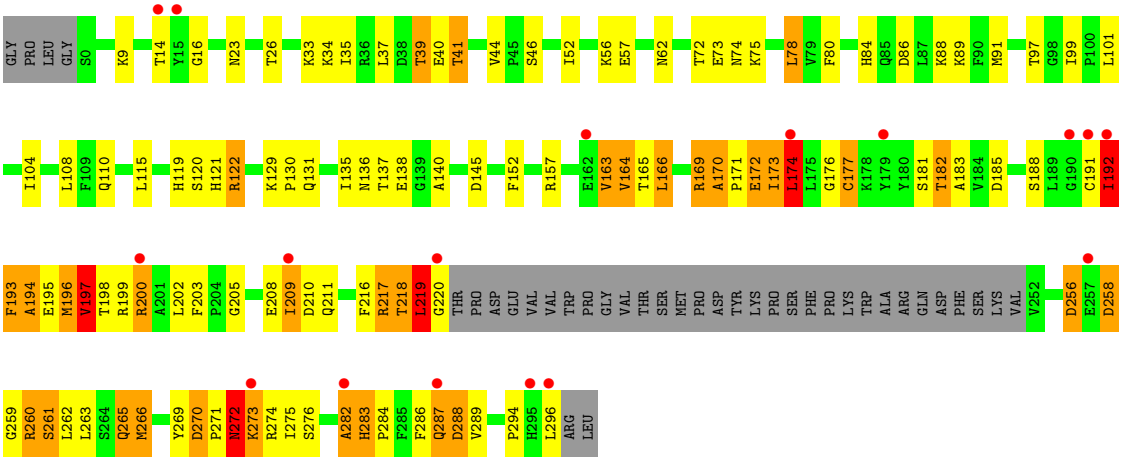
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A:



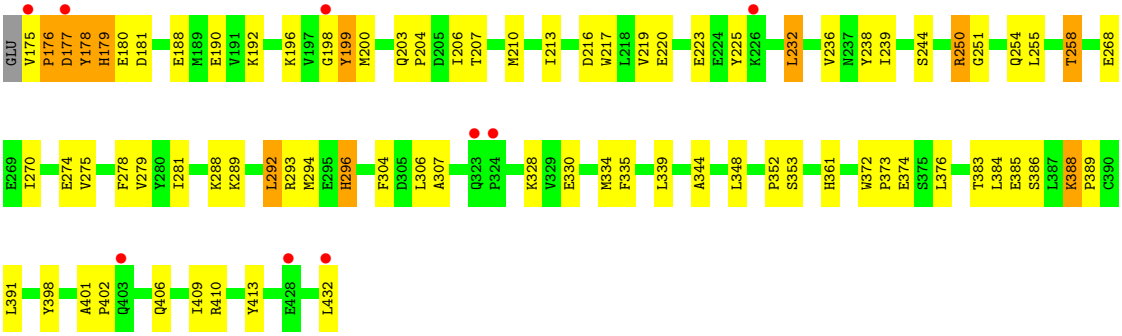
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain C:

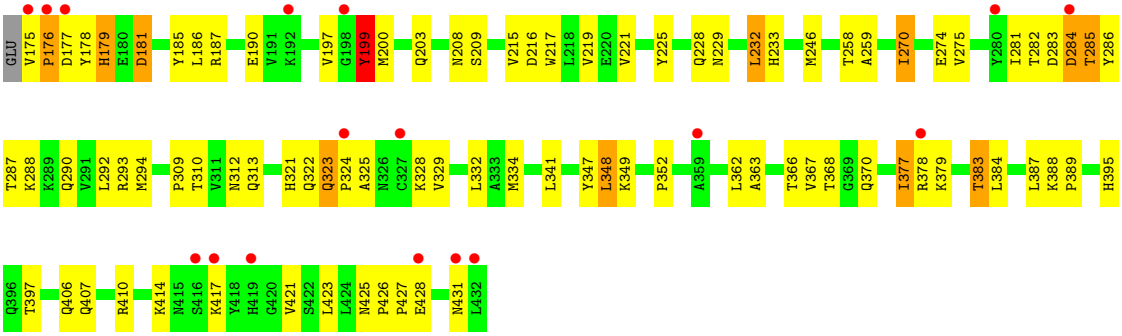


• Molecule 2: CYCLIN-A2

Chain B:



• Molecule 2: CYCLIN-A2



• Molecule 3: CYCLIC RKLFN-NH2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.79Å 131.85Å 146.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.80 24.43 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (100.00-2.80) 99.6 (24.43-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.285 0.211 , 0.283	Depositor DCC
R_{free} test set	1764 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	47.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8827	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: 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	0.55	0/2438	0.67	0/3308
1	C	0.55	0/2168	0.84	4/2935 (0.1%)
2	B	0.51	0/2133	0.65	0/2897
2	D	0.48	0/2133	0.62	1/2897 (0.0%)
3	E	0.48	0/47	0.78	0/60
All	All	0.52	0/8919	0.70	5/12097 (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	A	0	1
1	C	0	2
2	B	0	1
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	272	ASN	N-CA-C	6.14	127.59	111.00
1	C	196	MET	C-N-CA	5.58	135.64	121.70
2	D	232	LEU	CA-CB-CG	5.54	128.03	115.30
1	C	265	GLN	N-CA-C	5.19	125.01	111.00
1	C	219	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	ILE	Peptide
2	B	176	PRO	Peptide
1	C	169	ARG	Peptide
1	C	260	ARG	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	2388	0	2430	95	0
1	C	2131	0	2178	126	0
2	B	2083	0	2107	62	0
2	D	2083	0	2107	62	0
3	E	47	0	49	5	0
4	A	32	0	0	3	0
4	B	32	0	0	5	0
4	C	15	0	0	0	0
4	D	16	0	0	2	0
All	All	8827	0	8871	327	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 19.

All (327) 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:260:ARG:N	1:C:261:SER:HB2	1.54	1.23
1:C:260:ARG:H	1:C:261:SER:CB	1.56	1.19
1:C:170:ALA:HB1	1:C:171:PRO:HA	1.25	1.17
1:C:287:GLN:CB	1:C:288:ASP:HB2	1.74	1.17
2:B:254:GLN:HG3	3:E:32:LEU:HD12	1.23	1.11
1:C:194:ALA:HB1	1:C:195:GLU:HB3	1.33	1.09
1:C:193:PHE:H	1:C:194:ALA:HB2	1.19	1.07
1:C:176:GLY:HA3	1:C:177:CYS:HB2	1.36	1.06
1:A:12:GLU:HB3	1:A:13:GLY:HA2	1.34	1.06
1:C:287:GLN:HB2	1:C:288:ASP:CB	1.83	1.06
1:C:194:ALA:HB3	1:C:196:MET:N	1.69	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:PHE:N	1:C:194:ALA:HB2	1.73	1.01
1:A:60:HIS:HD2	1:A:62:ASN:H	1.09	0.99
1:C:284:PRO:O	1:C:287:GLN:HG2	1.66	0.96
1:C:272:ASN:H	1:C:274:ARG:H	1.14	0.94
1:C:287:GLN:HB2	1:C:288:ASP:HB2	0.97	0.94
1:C:260:ARG:H	1:C:261:SER:HB2	0.78	0.92
1:C:217:ARG:HG3	1:C:217:ARG:HH11	1.38	0.88
1:A:14:THR:HG22	1:A:15:TYR:H	1.36	0.88
1:A:150:ARG:NH2	2:B:268:GLU:O	2.05	0.88
1:C:176:GLY:CA	1:C:177:CYS:HB2	2.03	0.87
1:C:194:ALA:HB3	1:C:195:GLU:C	1.95	0.87
1:C:170:ALA:HB1	1:C:171:PRO:CA	2.05	0.86
1:C:176:GLY:HA3	1:C:177:CYS:CB	2.04	0.86
1:C:272:ASN:N	1:C:274:ARG:H	1.74	0.85
1:A:9:LYS:HD3	1:A:9:LYS:H	1.42	0.84
1:C:194:ALA:CB	1:C:195:GLU:HB3	2.07	0.84
1:C:169:ARG:HH11	1:C:174:LEU:HD22	1.43	0.83
1:A:12:GLU:CB	1:A:13:GLY:HA2	2.07	0.81
2:D:284:ASP:HA	2:D:286:TYR:H	1.46	0.79
1:A:88:LYS:HD2	1:A:131:GLN:HE21	1.48	0.79
1:A:291:LYS:HB3	4:A:2032:HOH:O	1.81	0.78
1:A:60:HIS:CD2	1:A:62:ASN:H	2.00	0.77
2:B:254:GLN:HG3	3:E:32:LEU:CD1	2.13	0.76
1:C:210:ASP:O	1:C:211:GLN:HB3	1.86	0.75
1:A:61:PRO:O	1:A:142:LYS:HE2	1.87	0.75
1:C:193:PHE:N	1:C:194:ALA:CB	2.50	0.74
1:C:193:PHE:O	1:C:193:PHE:CD1	2.41	0.74
1:A:160:TPO:HG22	2:B:270:ILE:HG23	1.70	0.73
1:C:129:LYS:HD3	1:C:165:THR:OG1	1.89	0.73
2:D:216:ASP:HB2	2:D:406:GLN:HG3	1.71	0.73
1:C:217:ARG:HH11	1:C:217:ARG:CG	2.01	0.72
1:C:194:ALA:HB3	1:C:195:GLU:CA	2.19	0.72
1:A:12:GLU:HB3	1:A:13:GLY:CA	2.15	0.72
1:A:133:LEU:HD11	1:A:192:ILE:HD13	1.71	0.72
1:C:287:GLN:CA	1:C:288:ASP:HB2	2.20	0.71
2:B:391:LEU:HD23	2:B:432:LEU:HD21	1.71	0.71
1:C:217:ARG:O	1:C:218:THR:OG1	2.06	0.70
1:C:262:LEU:O	1:C:265:GLN:HB2	1.90	0.70
2:D:284:ASP:HA	2:D:286:TYR:N	2.06	0.70
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.73	0.70
1:A:121:HIS:O	1:A:122:ARG:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ALA:HA	1:C:283:HIS:O	1.91	0.69
2:B:216:ASP:HB2	2:B:406:GLN:HG2	1.76	0.67
2:B:177:ASP:HB3	2:B:178:TYR:CD2	2.30	0.67
1:A:83:LEU:HD21	1:A:142:LYS:HD2	1.77	0.67
2:D:384:LEU:HA	2:D:387:LEU:HB2	1.76	0.67
1:C:131:GLN:N	1:C:131:GLN:OE1	2.28	0.67
1:C:194:ALA:H	1:C:197:VAL:HG11	1.61	0.66
1:A:249:SER:HA	1:A:260:ARG:HD3	1.78	0.65
1:A:178:LYS:H	1:A:178:LYS:HD3	1.61	0.65
1:A:150:ARG:NH1	1:A:160:TPO:O2P	2.30	0.65
1:C:99:ILE:HD12	1:C:196:MET:O	1.97	0.64
2:D:395:HIS:HE1	2:D:427:PRO:O	1.79	0.64
2:B:190:GLU:OE2	2:B:353:SER:N	2.24	0.64
2:D:270:ILE:HD13	2:D:270:ILE:H	1.62	0.64
2:B:190:GLU:HG2	2:B:352:PRO:HD2	1.79	0.64
1:C:194:ALA:CB	1:C:195:GLU:CA	2.75	0.64
1:A:39:THR:OG1	2:B:292:LEU:HD23	1.98	0.63
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.81	0.63
1:A:227:TRP:O	1:A:230:VAL:HG22	1.98	0.63
1:C:191:CYS:N	1:C:192:ILE:O	2.32	0.63
2:D:270:ILE:HG12	4:D:2009:HOH:O	1.99	0.63
1:C:272:ASN:H	1:C:274:ARG:N	1.90	0.63
1:C:115:LEU:HD11	1:C:185:ASP:HB3	1.81	0.62
1:C:219:LEU:HD11	1:C:269:TYR:HB2	1.80	0.62
2:B:344:ALA:O	2:B:348:LEU:HB2	1.99	0.62
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.81	0.61
2:D:384:LEU:HD12	2:D:384:LEU:H	1.65	0.61
1:C:194:ALA:CB	1:C:195:GLU:CB	2.77	0.61
2:B:207:THR:OG1	2:B:210:MET:HG3	2.01	0.61
1:A:178:LYS:H	1:A:178:LYS:CD	2.13	0.61
1:C:169:ARG:HH11	1:C:174:LEU:CD2	2.11	0.61
1:C:120:SER:HB2	1:C:121:HIS:HD2	1.66	0.60
1:A:242:LYS:HE3	4:A:2024:HOH:O	2.02	0.59
2:B:177:ASP:HB2	4:B:2001:HOH:O	2.03	0.59
1:C:261:SER:O	1:C:265:GLN:HG3	2.01	0.59
1:A:71:HIS:CE1	2:B:304:PHE:HE2	2.20	0.59
1:C:108:LEU:HD22	1:C:193:PHE:CD1	2.38	0.59
2:D:368:THR:HG23	2:D:370:GLN:H	1.67	0.59
2:B:384:LEU:HD12	4:B:2026:HOH:O	2.03	0.58
1:A:95:ALA:HA	1:A:199:ARG:HH11	1.69	0.58
1:A:14:THR:O	1:A:15:TYR:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:GLN:CG	3:E:32:LEU:HD12	2.16	0.58
1:C:16:GLY:HA3	1:C:34:LYS:O	2.03	0.58
1:A:157:ARG:HH22	2:B:268:GLU:HG3	1.69	0.57
1:C:188:SER:O	1:C:191:CYS:HB2	2.04	0.57
1:A:231:THR:HA	1:A:236:TYR:CD1	2.39	0.57
2:D:190:GLU:OE2	2:D:352:PRO:HD2	2.04	0.57
1:A:172:GLU:HG2	1:A:271:PRO:HG3	1.86	0.57
1:A:15:TYR:HD1	1:A:35:ILE:HG12	1.68	0.57
1:C:40:GLU:O	2:D:288:LYS:HD3	2.04	0.57
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.86	0.57
1:C:170:ALA:CB	1:C:171:PRO:HA	2.15	0.57
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.86	0.57
2:B:289:LYS:O	2:B:293:ARG:HG3	2.05	0.56
1:A:170:ALA:HB1	1:A:172:GLU:OE2	2.06	0.56
2:D:368:THR:HG23	2:D:370:GLN:HB2	1.87	0.56
2:D:287:THR:OG1	2:D:290:GLN:HG3	2.06	0.56
2:D:407:GLN:OE1	2:D:410:ARG:HD3	2.06	0.56
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.71	0.55
2:D:366:THR:HG23	2:D:427:PRO:HD3	1.87	0.55
1:A:59:ASN:OD1	1:A:65:LYS:HE2	2.07	0.55
2:D:221:VAL:HG22	2:D:281:ILE:HG21	1.88	0.55
1:C:270:ASP:OD1	1:C:273:LYS:HG2	2.07	0.55
1:A:2:GLU:HG2	1:C:73:GLU:OE1	2.07	0.54
1:C:194:ALA:HB3	1:C:196:MET:H	1.65	0.54
2:D:181:ASP:OD1	2:D:181:ASP:N	2.41	0.54
1:A:156:VAL:HG22	2:B:175:VAL:HG21	1.90	0.54
1:C:199:ARG:HG2	1:C:200:ARG:N	2.22	0.54
2:D:282:THR:O	2:D:285:THR:OG1	2.26	0.54
2:D:309:PRO:HA	2:D:313:GLN:NE2	2.22	0.54
1:C:262:LEU:HB2	1:C:283:HIS:CE1	2.43	0.54
2:D:176:PRO:HA	2:D:179:HIS:CE1	2.42	0.53
2:D:197:VAL:HG23	2:D:349:LYS:HB3	1.89	0.53
1:C:183:ALA:CB	1:C:271:PRO:HB3	2.38	0.53
1:C:260:ARG:N	1:C:261:SER:CB	2.37	0.53
1:A:60:HIS:HD2	1:A:62:ASN:N	1.91	0.53
1:C:119:HIS:CG	1:C:182:THR:OG1	2.62	0.53
2:D:197:VAL:CG2	2:D:349:LYS:HB3	2.38	0.53
1:C:256:ASP:OD1	1:C:256:ASP:N	2.41	0.53
1:C:173:ILE:HG22	1:C:174:LEU:HB2	1.90	0.53
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.44	0.52
1:C:39:THR:C	1:C:41:THR:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:VAL:HG11	2:B:292:LEU:HD13	1.90	0.52
2:B:373:PRO:HD2	2:B:376:LEU:HD12	1.91	0.52
1:C:192:ILE:HA	1:C:194:ALA:HB2	1.91	0.52
2:D:176:PRO:O	2:D:178:TYR:N	2.40	0.52
2:D:259:ALA:CB	2:D:294:MET:HG3	2.40	0.52
1:C:219:LEU:HD13	1:C:220:GLY:H	1.72	0.52
1:A:62:ASN:HA	1:A:142:LYS:HG2	1.92	0.52
2:B:238:TYR:CZ	2:B:306:LEU:HD22	2.45	0.52
1:A:71:HIS:NE2	2:B:296:HIS:ND1	2.57	0.52
2:D:233:HIS:CD2	2:D:341:LEU:HD21	2.44	0.52
2:D:347:TYR:HH	2:D:397:THR:HG1	1.57	0.52
1:C:121:HIS:O	1:C:122:ARG:HG3	2.09	0.52
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.90	0.52
1:C:170:ALA:CB	1:C:171:PRO:CA	2.79	0.51
2:B:199:TYR:HB2	2:B:244:SER:HA	1.92	0.51
2:D:186:LEU:HD22	2:D:309:PRO:HB3	1.91	0.51
2:D:323:GLN:HA	2:D:324:PRO:C	2.31	0.51
1:A:107:TYR:O	1:A:111:LEU:HG	2.10	0.51
1:C:157:ARG:HD2	2:D:228:GLN:OE1	2.11	0.51
1:C:193:PHE:N	1:C:194:ALA:CA	2.74	0.51
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.79	0.51
2:B:179:HIS:CD2	2:B:180:GLU:H	2.29	0.51
1:C:172:GLU:O	1:C:177:CYS:CB	2.59	0.51
1:C:192:ILE:N	1:C:194:ALA:HB1	2.26	0.51
1:A:293:VAL:HG12	1:A:294:PRO:O	2.11	0.50
2:B:188:GLU:CB	4:B:2005:HOH:O	2.59	0.50
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.93	0.50
2:B:236:VAL:HA	2:B:239:ILE:HD12	1.93	0.50
1:C:173:ILE:CG2	1:C:174:LEU:HB2	2.42	0.50
1:C:86:ASP:HB2	1:C:89:LYS:H	1.76	0.50
1:A:13:GLY:HA3	1:A:14:THR:C	2.32	0.50
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.93	0.50
1:A:121:HIS:C	1:A:122:ARG:HG3	2.31	0.50
1:C:199:ARG:HG2	1:C:200:ARG:H	1.77	0.50
1:A:50:ARG:NH1	1:A:160:TPO:O3P	2.39	0.50
1:C:272:ASN:N	1:C:274:ARG:N	2.52	0.49
1:C:196:MET:N	1:C:197:VAL:HG12	2.27	0.49
2:D:323:GLN:HA	2:D:325:ALA:N	2.27	0.49
2:B:217:TRP:HH2	2:B:258:THR:HG23	1.76	0.49
1:A:258:ASP:HB3	1:A:285:PHE:HA	1.95	0.49
1:C:194:ALA:CB	1:C:196:MET:N	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLN:HE22	1:A:22:ARG:NH2	2.10	0.49
1:A:39:THR:HG23	1:A:41:THR:H	1.78	0.49
1:C:193:PHE:CD1	1:C:193:PHE:C	2.84	0.49
2:D:347:TYR:C	2:D:349:LYS:H	2.16	0.49
1:C:193:PHE:O	1:C:193:PHE:HD1	1.94	0.48
1:A:71:HIS:HE1	2:B:304:PHE:CE2	2.32	0.48
1:C:217:ARG:HG3	1:C:217:ARG:NH1	2.18	0.48
1:C:23:ASN:HB3	1:C:26:THR:OG1	2.13	0.48
2:B:383:THR:OG1	2:B:385:GLU:HB3	2.14	0.48
1:A:71:HIS:CE1	2:B:304:PHE:CE2	3.01	0.48
2:B:278:PHE:HA	2:B:281:ILE:HG12	1.95	0.48
1:A:36:ARG:NH1	1:A:36:ARG:HB3	2.29	0.47
1:A:230:VAL:C	1:A:232:SER:H	2.16	0.47
2:D:414:LYS:HG2	2:D:423:LEU:HG	1.96	0.47
1:A:256:ASP:O	1:A:257:GLU:CB	2.61	0.47
1:C:84:HIS:HB3	1:C:135:ILE:O	2.14	0.47
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.49	0.47
1:A:15:TYR:CD1	1:A:35:ILE:HG12	2.48	0.47
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.50	0.47
2:B:361:HIS:HD2	2:B:391:LEU:HD21	1.80	0.47
1:C:52:ILE:O	1:C:56:LYS:HB2	2.15	0.47
2:B:279:VAL:HG21	2:B:288:LYS:HG3	1.97	0.47
1:C:72:THR:HB	1:C:75:LYS:H	1.80	0.47
1:C:91:MET:CE	1:C:195:GLU:HG2	2.45	0.47
1:A:9:LYS:H	1:A:9:LYS:CD	2.21	0.46
1:A:288:ASP:HB3	4:A:2029:HOH:O	2.15	0.46
1:A:284:PRO:O	1:A:287:GLN:HG2	2.15	0.46
1:C:33:LYS:HD3	1:C:80:PHE:HE1	1.79	0.46
1:C:209:ILE:HG13	1:C:210:ASP:N	2.29	0.46
2:D:347:TYR:OH	2:D:397:THR:OG1	2.30	0.46
1:C:35:ILE:HD12	1:C:78:LEU:HD21	1.96	0.46
1:A:71:HIS:CD2	2:B:296:HIS:CE1	3.03	0.46
1:A:137:THR:O	1:A:293:VAL:HG13	2.16	0.46
1:C:203:PHE:HB2	1:C:211:GLN:HE22	1.79	0.46
1:C:265:GLN:HB3	1:C:275:ILE:HB	1.96	0.46
2:D:425:ASN:OD1	2:D:426:PRO:HD2	2.16	0.46
2:B:198:GLY:O	2:B:200:MET:N	2.48	0.46
1:C:208:GLU:O	1:C:209:ILE:HG12	2.16	0.46
2:D:312:ASN:ND2	2:D:334:MET:SD	2.89	0.46
1:A:7:VAL:HG12	1:A:8:GLU:HG2	1.98	0.46
1:C:163:VAL:HG13	1:C:164:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:282:THR:C	2:D:284:ASP:H	2.18	0.46
1:A:14:THR:HG22	1:A:15:TYR:N	2.17	0.46
1:A:40:GLU:C	1:A:42:GLU:H	2.18	0.45
1:A:51:GLU:O	1:A:55:LEU:HB2	2.16	0.45
1:C:197:VAL:HG13	1:C:198:THR:HG23	1.97	0.45
1:A:122:ARG:NH2	2:B:307:ALA:HB1	2.32	0.45
3:E:31:LYS:HD3	3:E:34:ASN:O	2.15	0.45
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.51	0.45
1:C:137:THR:HG22	1:C:137:THR:O	2.15	0.45
1:A:223:ASP:H	1:A:226:VAL:HG12	1.81	0.45
2:B:372:TRP:CZ2	2:B:376:LEU:HB3	2.52	0.45
2:D:215:VAL:O	2:D:219:VAL:HG23	2.16	0.45
1:C:173:ILE:HB	1:C:174:LEU:HB2	1.98	0.45
1:C:270:ASP:HA	1:C:271:PRO:HD3	1.82	0.45
2:B:177:ASP:N	2:B:179:HIS:H	2.15	0.45
1:C:202:LEU:HD13	1:C:203:PHE:CZ	2.52	0.45
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.99	0.45
2:D:282:THR:O	2:D:284:ASP:N	2.51	0.44
1:A:55:LEU:HD22	1:A:146:PHE:HB2	1.99	0.44
2:B:219:VAL:HG21	2:B:409:ILE:HG13	1.98	0.44
2:B:391:LEU:HD23	2:B:432:LEU:CD2	2.45	0.44
2:D:384:LEU:HD12	2:D:384:LEU:N	2.31	0.44
1:A:9:LYS:HD3	1:A:9:LYS:N	2.21	0.44
2:D:310:THR:OG1	2:D:313:GLN:HG3	2.17	0.44
1:A:40:GLU:OE1	1:A:43:GLY:O	2.34	0.44
1:A:105:LYS:HG2	1:A:285:PHE:CZ	2.52	0.44
2:D:225:TYR:CE1	2:D:281:ILE:HD11	2.52	0.44
1:C:294:PRO:HG2	1:C:296:LEU:HD21	2.00	0.44
1:C:170:ALA:HA	1:C:171:PRO:O	2.18	0.44
2:D:200:MET:HG2	2:D:208:ASN:N	2.33	0.44
2:D:229:ASN:ND2	4:D:2003:HOH:O	2.51	0.44
2:D:199:TYR:CE2	2:D:348:LEU:HD21	2.52	0.44
2:B:401:ALA:HB1	2:B:410:ARG:HD2	2.00	0.44
1:A:52:ILE:HD11	1:A:78:LEU:HD21	2.00	0.43
1:A:104:ILE:HG23	1:A:196:MET:HE3	2.00	0.43
1:A:256:ASP:O	1:A:257:GLU:HB2	2.18	0.43
1:C:37:LEU:HD22	1:C:44:VAL:HG22	1.99	0.43
1:C:194:ALA:H	1:C:197:VAL:CG1	2.28	0.43
1:C:192:ILE:HA	1:C:194:ALA:CB	2.47	0.43
1:C:181:SER:OG	1:C:182:THR:N	2.48	0.43
1:A:227:TRP:CE3	1:A:269:TYR:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLN:HE21	1:A:5:GLN:HB3	1.46	0.43
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.34	0.43
1:C:169:ARG:HD2	1:C:174:LEU:HD22	1.99	0.43
1:A:14:THR:O	1:A:15:TYR:CB	2.67	0.43
1:C:172:GLU:O	1:C:177:CYS:HB3	2.18	0.43
1:A:9:LYS:C	1:A:10:ILE:HG13	2.40	0.42
1:A:136:ASN:ND2	1:A:140:ALA:HB3	2.34	0.42
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.34	0.42
2:D:377:ILE:HD13	2:D:383:THR:HG22	2.01	0.42
1:A:115:LEU:HD23	1:A:186:ILE:HD13	2.00	0.42
2:B:188:GLU:HB2	4:B:2005:HOH:O	2.19	0.42
2:B:196:LYS:HE3	2:B:199:TYR:HA	2.01	0.42
2:D:217:TRP:CH2	2:D:282:THR:HG22	2.54	0.42
2:B:330:GLU:O	2:B:334:MET:HG2	2.19	0.42
1:C:91:MET:HE1	1:C:195:GLU:HG2	2.01	0.42
1:C:258:ASP:HA	1:C:259:GLY:HA2	1.73	0.42
1:A:7:VAL:HB	1:A:20:LYS:HG2	2.01	0.42
2:D:175:VAL:HA	2:D:176:PRO:HD3	1.72	0.42
1:C:78:LEU:HD23	1:C:78:LEU:N	2.34	0.42
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.02	0.42
1:C:101:LEU:HA	1:C:104:ILE:HD12	2.01	0.42
2:B:216:ASP:HB2	2:B:406:GLN:CG	2.47	0.42
1:C:121:HIS:C	1:C:122:ARG:HG3	2.40	0.42
2:D:203:GLN:NE2	2:D:246:MET:O	2.48	0.42
1:C:171:PRO:C	1:C:173:ILE:H	2.23	0.42
1:A:25:LEU:HD21	2:D:293:ARG:HB2	2.01	0.42
1:C:157:ARG:CZ	2:D:228:GLN:HG3	2.50	0.41
2:D:199:TYR:CD2	2:D:348:LEU:HD21	2.55	0.41
2:D:329:VAL:HG23	2:D:367:VAL:HB	2.02	0.41
1:C:216:PHE:HD1	1:C:219:LEU:HB3	1.85	0.41
2:B:250:ARG:HG3	2:B:251:GLY:N	2.35	0.41
1:C:171:PRO:O	1:C:173:ILE:N	2.54	0.41
1:C:172:GLU:O	1:C:177:CYS:HB2	2.20	0.41
1:A:33:LYS:HB3	1:A:78:LEU:HB2	2.02	0.41
1:A:241:PRO:HB2	1:A:243:TRP:CH2	2.55	0.41
2:B:213:ILE:HG22	3:E:32:LEU:HD22	2.02	0.41
2:B:274:GLU:H	2:B:274:GLU:HG2	1.66	0.41
1:C:259:GLY:HA3	1:C:262:LEU:HB3	2.02	0.41
2:D:321:HIS:CE1	2:D:379:LYS:HD2	2.56	0.41
2:D:328:LYS:O	2:D:421:VAL:HG11	2.21	0.41
1:A:101:LEU:N	1:A:102:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:LEU:CD2	2:B:432:LEU:HD21	2.44	0.41
1:C:39:THR:O	1:C:41:THR:N	2.51	0.41
1:C:205:GLY:HA3	1:C:211:GLN:HB2	2.02	0.41
1:C:263:LEU:C	1:C:265:GLN:H	2.23	0.41
1:C:57:GLU:CG	2:D:185:TYR:OH	2.68	0.41
1:A:230:VAL:C	1:A:232:SER:N	2.74	0.41
2:B:339:LEU:HD23	2:B:339:LEU:HA	1.94	0.41
1:C:91:MET:HE2	1:C:196:MET:HA	2.02	0.41
1:C:173:ILE:CB	1:C:174:LEU:HB2	2.51	0.41
1:A:25:LEU:HD11	2:D:293:ARG:HB3	2.03	0.41
1:A:95:ALA:HA	1:A:199:ARG:NH1	2.36	0.41
1:A:252:VAL:HG11	1:A:255:LEU:HD22	2.01	0.41
1:C:266:MET:N	1:C:275:ILE:HG22	2.35	0.41
2:D:187:ARG:HD2	2:D:187:ARG:HA	1.78	0.41
1:A:163:VAL:CG1	1:A:164:VAL:HG23	2.51	0.41
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.86	0.40
2:B:188:GLU:HB3	4:B:2005:HOH:O	2.20	0.40
1:A:65:LYS:H	1:A:81:GLU:HG2	1.86	0.40
1:A:171:PRO:HD3	1:A:187:TRP:CE2	2.56	0.40
2:B:203:GLN:HA	2:B:204:PRO:HD2	1.95	0.40
2:B:255:LEU:HG	2:B:294:MET:HG2	2.02	0.40
2:D:258:THR:OG1	2:D:282:THR:HG21	2.22	0.40
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.57	0.40
2:B:203:GLN:HB3	2:B:206:ILE:HG12	2.04	0.40
1:C:203:PHE:HB2	1:C:211:GLN:NE2	2.37	0.40
1:C:286:PHE:O	1:C:287:GLN:C	2.59	0.40
1:A:268:HIS:NE2	1:A:273:LYS:HD2	2.37	0.40
2:D:270:ILE:H	2:D:270:ILE:CD1	2.29	0.40
2:D:275:VAL:HG21	2:D:292:LEU:HD21	2.03	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	294/303 (97%)	266 (90%)	21 (7%)	7 (2%)	6 20
1	C	261/303 (86%)	204 (78%)	34 (13%)	23 (9%)	1 1
2	B	256/259 (99%)	240 (94%)	12 (5%)	4 (2%)	9 31
2	D	256/259 (99%)	233 (91%)	14 (6%)	9 (4%)	3 12
3	E	3/5 (60%)	2 (67%)	1 (33%)	0	100 100
All	All	1070/1129 (95%)	945 (88%)	82 (8%)	43 (4%)	3 9

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	TYR
2	B	176	PRO
1	C	170	ALA
1	C	177	CYS
1	C	192	ILE
1	C	256	ASP
2	D	176	PRO
2	D	177	ASP
2	D	284	ASP
2	D	322	GLN
1	A	95	ALA
1	A	257	GLU
2	B	177	ASP
1	C	164	VAL
1	C	173	ILE
1	C	193	PHE
1	C	194	ALA
1	C	218	THR
1	C	287	GLN
1	C	288	ASP
2	D	283	ASP
2	D	285	THR
1	A	12	GLU
1	A	41	THR
1	A	164	VAL
2	B	178	TYR
1	C	197	VAL
1	C	266	MET
1	C	272	ASN
1	C	273	LYS
1	C	282	ALA

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Mol	Chain	Res	Type
1	C	283	HIS
2	D	199	TYR
2	D	348	LEU
1	C	200	ARG
1	C	261	SER
2	D	323	GLN
1	A	10	ILE
1	C	145	ASP
1	C	166	LEU
1	C	174	LEU
1	C	258	ASP
2	B	388	LYS

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%)	236 (90%)	25 (10%)	8 24
1	C	231/265 (87%)	208 (90%)	23 (10%)	7 22
2	B	232/233 (100%)	217 (94%)	15 (6%)	17 44
2	D	232/233 (100%)	218 (94%)	14 (6%)	19 48
3	E	5/5 (100%)	5 (100%)	0	100 100
All	All	961/1001 (96%)	884 (92%)	77 (8%)	12 34

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	9	LYS
1	A	10	ILE
1	A	14	THR
1	A	17	VAL
1	A	19	TYR
1	A	36	ARG

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Mol	Chain	Res	Type
1	A	38	ASP
1	A	39	THR
1	A	40	GLU
1	A	47	THR
1	A	55	LEU
1	A	73	GLU
1	A	94	SER
1	A	101	LEU
1	A	122	ARG
1	A	128	LEU
1	A	148	LEU
1	A	163	VAL
1	A	178	LYS
1	A	206	ASP
1	A	230	VAL
1	A	232	SER
1	A	256	ASP
1	A	272	ASN
2	B	179	HIS
2	B	181	ASP
2	B	192	LYS
2	B	199	TYR
2	B	220	GLU
2	B	223	GLU
2	B	232	LEU
2	B	250	ARG
2	B	258	THR
2	B	292	LEU
2	B	296	HIS
2	B	328	LYS
2	B	374	GLU
2	B	386	SER
2	B	398	TYR
1	C	9	LYS
1	C	14	THR
1	C	39	THR
1	C	41	THR
1	C	46	SER
1	C	74	ASN
1	C	78	LEU
1	C	97	THR
1	C	122	ARG

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Mol	Chain	Res	Type
1	C	138	GLU
1	C	163	VAL
1	C	166	LEU
1	C	172	GLU
1	C	174	LEU
1	C	182	THR
1	C	192	ILE
1	C	197	VAL
1	C	209	ILE
1	C	217	ARG
1	C	219	LEU
1	C	270	ASP
1	C	276	SER
1	C	289	VAL
2	D	179	HIS
2	D	181	ASP
2	D	199	TYR
2	D	209	SER
2	D	232	LEU
2	D	270	ILE
2	D	274	GLU
2	D	362	LEU
2	D	377	ILE
2	D	378	ARG
2	D	383	THR
2	D	417	LYS
2	D	428	GLU
2	D	431	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	60	HIS
1	A	85	GLN
2	B	179	HIS
2	B	370	GLN
1	C	121	HIS
1	C	268	HIS
2	D	254	GLN
2	D	312	ASN
2	D	313	GLN

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Mol	Chain	Res	Type
2	D	370	GLN
2	D	395	HIS
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	C	160	1	8,10,11	0.88	0	10,14,16	1.18	0
1	TPO	A	160	1	8,10,11	0.98	0	10,14,16	1.45	2 (20%)

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	C	160	1	-	0/9/11/13	-
1	TPO	A	160	1	-	6/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	160	TPO	O3P-P-O2P	2.28	116.33	107.64
1	A	160	TPO	P-OG1-CB	2.11	129.59	123.21

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	N-CA-CB-CG2
1	A	160	TPO	N-CA-CB-OG1
1	A	160	TPO	C-CA-CB-CG2
1	A	160	TPO	O-C-CA-CB
1	A	160	TPO	CG2-CB-OG1-P
1	A	160	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	160	TPO	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 (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^{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	296/303 (97%)	-0.19	8 (2%) 54 44	22, 35, 67, 79	0
1	C	265/303 (87%)	0.26	17 (6%) 19 12	32, 53, 78, 83	0
2	B	258/259 (99%)	-0.01	9 (3%) 44 34	25, 39, 55, 65	0
2	D	258/259 (99%)	0.27	17 (6%) 18 11	30, 53, 82, 93	0
3	E	5/5 (100%)	0.94	1 (20%) 1 0	62, 63, 68, 71	0
All	All	1082/1129 (95%)	0.08	52 (4%) 30 21	22, 44, 78, 93	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	432	LEU	6.2
1	C	296	LEU	5.3
2	B	324	PRO	3.8
3	E	34	ASN	3.8
1	C	287	GLN	3.7
1	A	95	ALA	3.7
1	C	220	GLY	3.6
1	C	174	LEU	3.6
1	A	38	ASP	3.5
1	A	96	LEU	3.5
2	D	419	HIS	3.5
2	B	226	LYS	3.4
1	A	162	GLU	3.4
1	C	14	THR	3.3
1	A	36	ARG	3.1
2	D	175	VAL	3.1
2	D	428	GLU	3.1
2	D	378	ARG	2.9
1	C	15	TYR	2.9
2	D	327	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	200	ARG	2.8
2	D	280	TYR	2.8
2	B	177	ASP	2.8
2	B	403	GLN	2.7
2	D	324	PRO	2.7
2	D	431	ASN	2.7
1	A	97	THR	2.6
2	D	417	LYS	2.6
1	C	282	ALA	2.5
1	C	162	GLU	2.5
1	C	295	HIS	2.4
2	D	192	LYS	2.4
2	D	198	GLY	2.4
2	D	416	SER	2.3
2	B	323	GLN	2.3
1	C	190	GLY	2.2
1	C	191	CYS	2.2
1	C	209	ILE	2.2
2	D	284	ASP	2.2
2	D	177	ASP	2.2
2	B	175	VAL	2.2
1	C	273	LYS	2.1
1	C	257	GLU	2.1
1	A	41	THR	2.1
1	C	192	ILE	2.1
2	B	432	LEU	2.1
2	D	359	ALA	2.1
2	B	198	GLY	2.1
1	C	179	TYR	2.0
1	A	74	ASN	2.0
2	B	428	GLU	2.0
2	D	176	PRO	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
1	TPO	C	160	11/12	0.95	0.16	50,53,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	A	160	11/12	0.97	0.13	39,41,42,42	0

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.