Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:05 PM GMT

PDB ID	:	3W2C
Title	:	Structure of Aurora kinase A complexed to benzoimidazole-indazole inhibitor XV
Authors	:	Oliveira, T.M.; Kairies, N.A.; Engh, R.A.
Deposited on	:	2012-11-28
Resolution	:	2.45 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

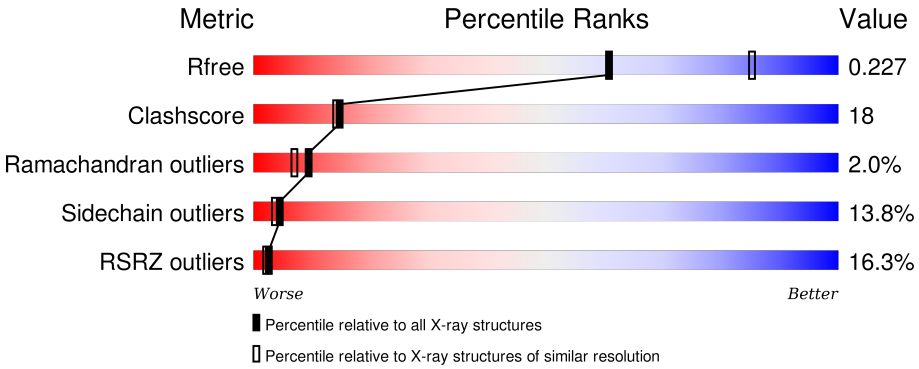
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 >=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 <=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	261	12% 47% 26% 5% 22%
1	C	261	11% 47% 24% 7% 23%
1	E	261	12% 50% 22% 5% 23%
1	G	261	16% 49% 25% 23%

2 Entry composition

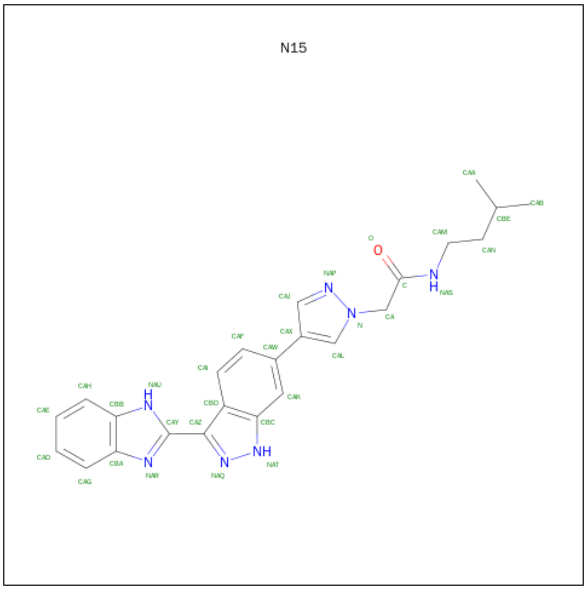
There are 3 unique types of molecules in this entry. The entry contains 6857 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aurora kinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1661	1085	275	298	3			
1	C	202	Total	C	N	O	S	0	0	0
			1645	1073	272	297	3			
1	E	202	Total	C	N	O	S	0	0	0
			1649	1076	273	297	3			
1	G	202	Total	C	N	O	S	0	0	0
			1649	1076	273	297	3			

- Molecule 2 is 2-{4-[3-(1H-BENZIMIDAZOL-2-YL)-1H-INDAZOL-6-YL]-1H-PYRAZOL-1-YL}-N-(3-METHYLBUTYL)ACETAMIDE (three-letter code: N15) (formula: $C_{24}H_{25}N_7O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	24	7	1		
2	C	1	Total	C	N	O	0	0
			32	24	7	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C N O 32 24 7 1	0	0
2	G	1	Total C N O 32 24 7 1	0	0

- Molecule 3 is water.

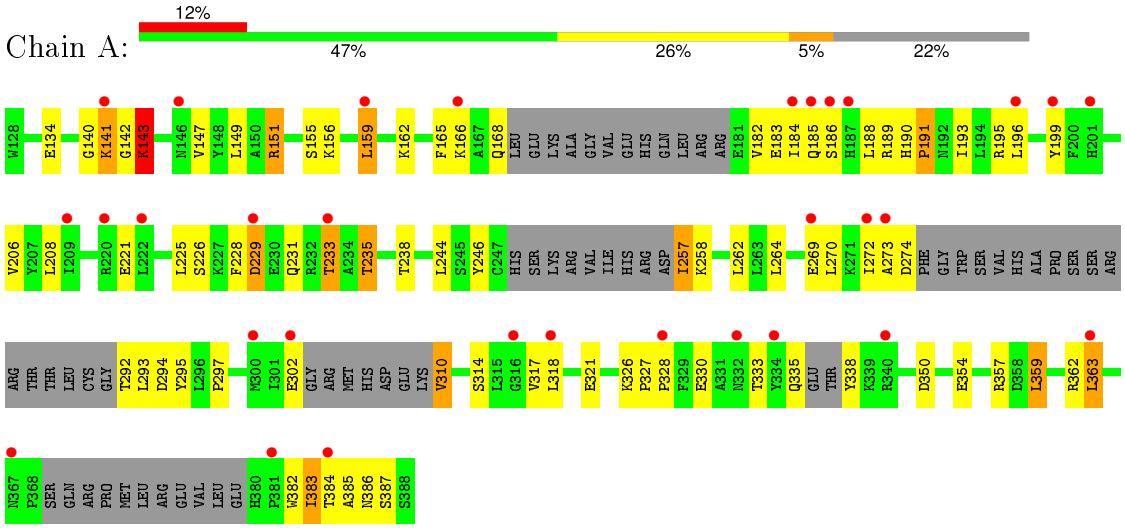
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	28	Total O 28 28	0	0
3	C	33	Total O 33 33	0	0
3	E	29	Total O 29 29	0	0
3	G	35	Total O 35 35	0	0

3 Residue-property plots (i)

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

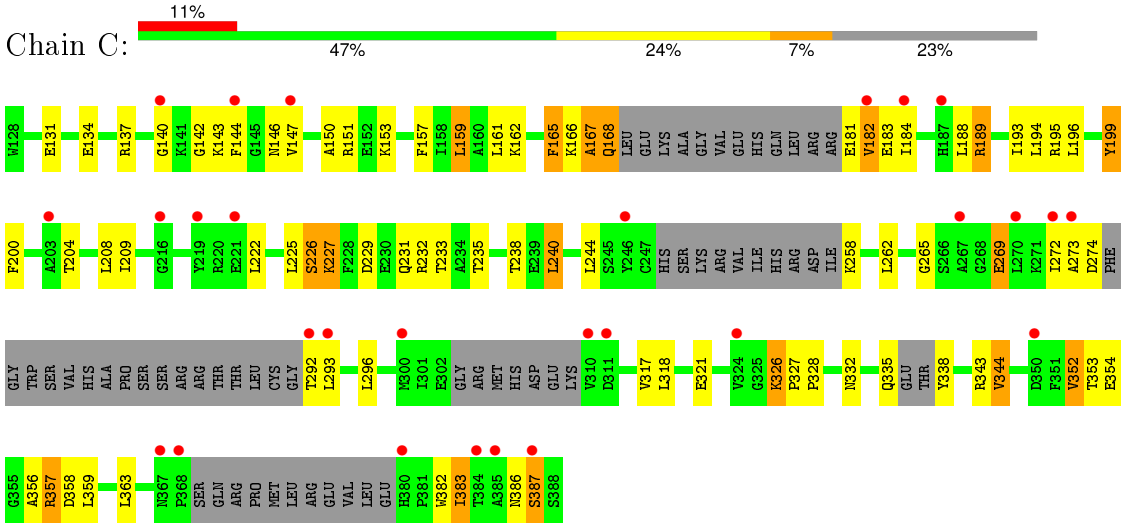
- Molecule 1: Aurora kinase A

Chain A:



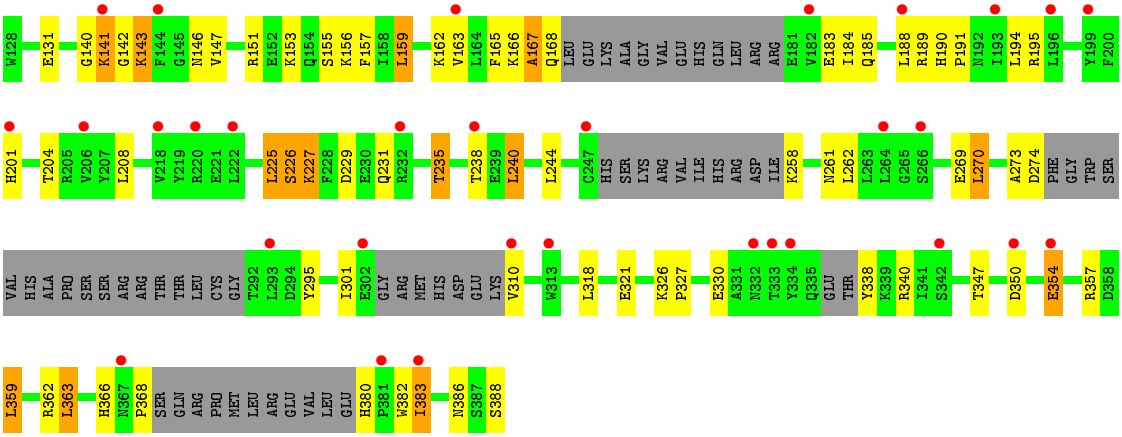
- Molecule 1: Aurora kinase A

Chain C:



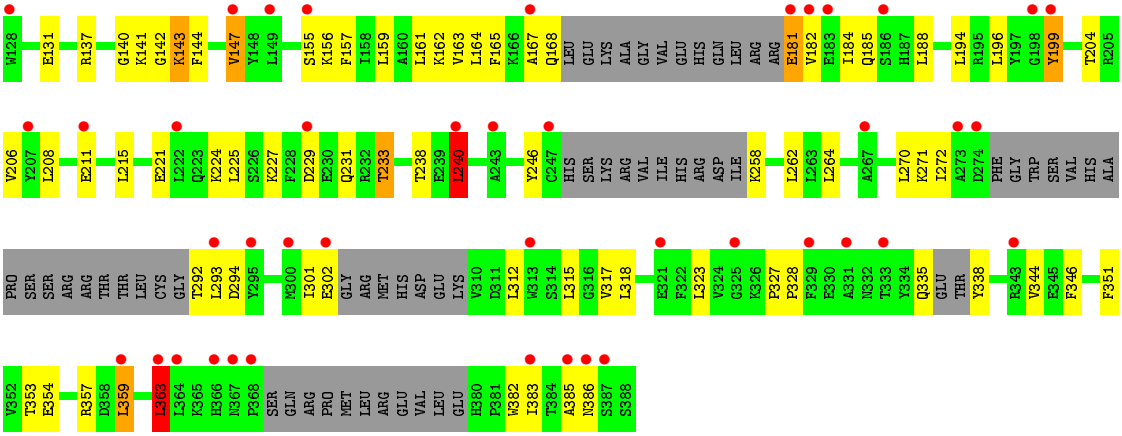
- Molecule 1: Aurora kinase A

Chain E:



- Molecule 1: Aurora kinase A

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.21Å 86.05Å 85.96Å 90.00° 89.83° 90.00°	Depositor
Resolution (Å)	45.73 – 2.45 45.73 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.5 (45.73-2.45) 92.9 (45.73-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.253 , 0.320 0.223 , 0.227	Depositor DCC
R_{free} test set	1816 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.2	EDS
Estimated twinning fraction	0.281 for H,K,L 0.242 for -H,L,K 0.249 for -H,-L,-K 0.229 for -H,-K,L 0.467 for -h,-l,-k 0.449 for -h,l,k 0.448 for h,-k,-l	Xtriage
Reported twinning fraction	0.281 for H,K,L 0.242 for -H,L,K 0.249 for -H,-L,-K 0.229 for -H,-K,L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 34812 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6857	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 4.36% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: N15

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	0.75	0/1699	0.87	2/2295 (0.1%)
1	C	0.77	0/1683	0.84	1/2276 (0.0%)
1	E	0.74	0/1687	0.82	1/2280 (0.0%)
1	G	0.71	0/1687	0.82	2/2280 (0.1%)
All	All	0.74	0/6756	0.84	6/9131 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	E	0	1
1	G	0	2
All	All	0	7

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	G	240	LEU	CA-CB-CG	6.44	130.11	115.30
1	E	159	LEU	CA-CB-CG	6.41	130.04	115.30
1	A	159	LEU	CA-CB-CG	6.24	129.66	115.30
1	C	140	GLY	N-CA-C	5.64	127.21	113.10
1	G	363	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	LYS	Peptide
1	A	350	ASP	Peptide
1	C	167	ALA	Peptide
1	C	387	SER	Peptide
1	E	143	LYS	Peptide
1	G	143	LYS	Peptide
1	G	181	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1661	0	1661	51	0
1	C	1645	0	1628	82	0
1	E	1649	0	1639	53	0
1	G	1649	0	1639	53	0
2	A	32	0	25	4	0
2	C	32	0	25	7	0
2	E	32	0	25	7	0
2	G	32	0	25	5	0
3	A	28	0	0	1	0
3	C	33	0	0	5	0
3	E	29	0	0	6	0
3	G	35	0	0	5	0
All	All	6857	0	6667	239	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (239) 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:167:ALA:CA	1:C:168:GLN:HG3	1.45	1.44
1:C:167:ALA:HB3	1:C:168:GLN:CD	1.46	1.35
1:C:167:ALA:HB3	1:C:168:GLN:CG	1.61	1.28

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ALA:CB	1:C:168:GLN:HG3	1.67	1.23
1:C:167:ALA:C	1:C:168:GLN:HG3	1.53	1.11
1:G:164:LEU:HB2	1:G:206:VAL:HG23	1.32	1.10
1:C:167:ALA:HB3	1:C:168:GLN:OE1	1.51	1.07
1:C:167:ALA:CB	1:C:168:GLN:CG	2.29	1.04
1:C:167:ALA:H	1:C:168:GLN:CB	1.69	1.04
1:C:167:ALA:CA	1:C:168:GLN:CG	2.35	1.04
1:C:165:PHE:O	1:C:167:ALA:HA	1.57	1.03
1:G:142:GLY:O	1:G:143:LYS:HG2	1.61	1.01
1:C:167:ALA:CB	1:C:168:GLN:CD	2.30	0.98
1:C:167:ALA:C	1:C:168:GLN:CG	2.34	0.95
1:E:231:GLN:O	1:E:235:THR:HG22	1.68	0.93
1:G:181:GLU:HG2	1:G:182:VAL:HG23	1.53	0.91
1:E:330:GLU:OE1	3:E:506:HOH:O	1.91	0.89
1:C:167:ALA:H	1:C:168:GLN:CA	1.85	0.89
1:A:140:GLY:O	1:A:142:GLY:N	2.04	0.88
1:C:167:ALA:N	1:C:168:GLN:C	2.30	0.85
1:A:162:LYS:HD3	2:A:401:N15:O	1.78	0.84
1:C:167:ALA:N	1:C:168:GLN:CA	2.36	0.84
1:G:164:LEU:HB2	1:G:206:VAL:CG2	2.07	0.84
1:E:380:HIS:CD2	1:E:382:TRP:H	1.97	0.82
1:C:167:ALA:N	1:C:168:GLN:HG3	1.94	0.81
1:C:167:ALA:N	1:C:168:GLN:CG	2.43	0.80
1:C:167:ALA:H	1:C:168:GLN:CG	1.95	0.79
1:E:231:GLN:O	1:E:235:THR:CG2	2.30	0.79
1:G:188:LEU:HG	1:G:246:TYR:HE2	1.49	0.77
1:G:140:GLY:O	1:G:142:GLY:N	2.17	0.77
1:C:167:ALA:N	1:C:168:GLN:CB	2.48	0.77
1:C:167:ALA:CB	1:C:168:GLN:OE1	2.29	0.77
1:C:231:GLN:O	1:C:235:THR:HG23	1.88	0.74
1:A:162:LYS:NZ	2:A:401:N15:H13	2.02	0.73
1:E:240:LEU:CD1	1:E:270:LEU:HD21	2.19	0.72
1:G:359:LEU:HD22	1:G:363:LEU:HD22	1.73	0.70
1:C:166:LYS:O	1:C:168:GLN:C	2.29	0.70
1:A:162:LYS:HB3	1:A:208:LEU:HB2	1.73	0.70
1:C:137:ARG:NH2	3:C:507:HOH:O	2.24	0.70
1:E:188:LEU:O	1:E:189:ARG:HG3	1.94	0.68
1:G:231:GLN:HA	1:G:386:ASN:O	1.93	0.67
1:A:193:ILE:HD13	1:A:272:ILE:HD11	1.77	0.67
1:E:340:ARG:NH1	3:E:504:HOH:O	2.27	0.66
1:G:240:LEU:HD21	1:G:318:LEU:HD23	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LYS:C	1:C:168:GLN:C	2.54	0.65
1:C:189:ARG:HD2	1:C:195:ARG:HD2	1.79	0.65
1:A:354:GLU:OE2	1:A:357:ARG:HD2	1.96	0.65
1:C:344:VAL:HG13	1:C:344:VAL:O	1.95	0.65
1:A:338:TYR:N	3:A:528:HOH:O	2.30	0.64
1:C:167:ALA:H	1:C:168:GLN:HB2	1.62	0.64
1:A:292:THR:HG23	1:A:293:LEU:H	1.62	0.64
1:E:359:LEU:HD22	1:E:363:LEU:HD22	1.81	0.63
1:A:327:PRO:HG2	1:A:330:GLU:HG3	1.81	0.63
1:G:385:ALA:HB2	3:G:519:HOH:O	1.98	0.63
1:E:240:LEU:HD11	1:E:270:LEU:HD21	1.81	0.62
1:C:167:ALA:H	1:C:168:GLN:C	1.97	0.62
1:G:262:LEU:HB3	1:G:270:LEU:CD1	2.30	0.62
1:C:162:LYS:HD2	1:C:208:LEU:HD12	1.82	0.61
1:E:240:LEU:HD13	1:E:270:LEU:HD21	1.83	0.61
1:A:189:ARG:HG2	1:A:195:ARG:HD3	1.81	0.61
1:A:195:ARG:HH21	1:A:195:ARG:HG3	1.66	0.61
1:G:258:LYS:N	3:G:529:HOH:O	2.34	0.61
1:C:131:GLU:O	1:C:153:LYS:HE3	2.01	0.61
1:A:228:PHE:HB2	1:A:233:THR:HG22	1.83	0.61
1:E:359:LEU:HD12	1:E:383:ILE:HD13	1.83	0.60
1:E:354:GLU:HA	1:E:357:ARG:HB2	1.83	0.60
1:C:157:PHE:CE2	1:C:159:LEU:HD13	2.37	0.60
1:G:162:LYS:HB3	1:G:208:LEU:HB2	1.84	0.59
1:C:142:GLY:O	1:C:144:PHE:N	2.34	0.59
1:G:262:LEU:HD11	1:G:318:LEU:HD21	1.86	0.58
1:C:194:LEU:CD2	2:C:401:N15:H16	2.34	0.58
1:E:380:HIS:CD2	1:E:382:TRP:N	2.72	0.57
1:A:162:LYS:HZ3	2:A:401:N15:H13	1.69	0.57
1:C:157:PHE:CE2	1:C:159:LEU:CD1	2.88	0.57
1:C:165:PHE:C	1:C:167:ALA:HA	2.24	0.56
1:G:292:THR:HG23	1:G:293:LEU:H	1.70	0.56
1:C:162:LYS:HE3	2:C:401:N15:O	2.06	0.56
1:E:162:LYS:HD2	1:E:208:LEU:HD12	1.87	0.56
1:C:343:ARG:O	1:C:344:VAL:HG12	2.05	0.56
1:G:211:GLU:OE2	1:G:271:LYS:HE3	2.06	0.56
1:A:190:HIS:ND1	1:A:191:PRO:HD2	2.21	0.56
1:C:134:GLU:HB2	1:C:151:ARG:HB3	1.88	0.56
1:A:166:LYS:HG3	1:A:206:VAL:HG23	1.88	0.55
1:G:335:GLN:O	1:G:338:TYR:HB3	2.06	0.55
1:E:167:ALA:O	1:E:168:GLN:O	2.25	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:LEU:HD11	1:E:318:LEU:HD21	1.88	0.55
1:G:155:SER:O	1:G:156:LYS:HB2	2.06	0.55
1:C:181:GLU:O	1:C:182:VAL:HB	2.07	0.54
1:G:233:THR:HG21	1:G:323:LEU:CD2	2.37	0.54
1:C:165:PHE:O	1:C:167:ALA:CA	2.44	0.54
1:C:338:TYR:N	3:C:512:HOH:O	2.41	0.54
1:E:235:THR:HB	1:E:388:SER:H	1.73	0.54
1:E:185:GLN:HA	1:E:188:LEU:HD13	1.90	0.53
1:C:144:PHE:C	1:C:146:ASN:H	2.10	0.53
1:A:262:LEU:HD11	1:A:318:LEU:HD21	1.90	0.53
1:G:182:VAL:O	1:G:182:VAL:HG12	2.07	0.53
1:C:352:VAL:HG23	1:C:356:ALA:HB3	1.91	0.53
1:G:317:VAL:HG13	1:G:328:PRO:HD2	1.90	0.53
1:C:293:LEU:HA	1:C:296:LEU:HD12	1.90	0.53
1:A:195:ARG:HG3	1:A:195:ARG:NH2	2.24	0.52
1:E:382:TRP:O	1:E:386:ASN:HB2	2.08	0.52
1:A:354:GLU:HA	1:A:357:ARG:HB2	1.91	0.52
1:C:240:LEU:HD21	1:C:318:LEU:HD23	1.90	0.52
1:E:184:ILE:HG13	1:E:185:GLN:N	2.24	0.52
1:E:194:LEU:CD2	2:E:401:N15:H16	2.39	0.52
1:A:162:LYS:HZ2	2:A:401:N15:H13	1.73	0.52
1:G:157:PHE:CD2	1:G:159:LEU:HD13	2.44	0.52
1:A:141:LYS:NZ	1:C:326:LYS:HZ2	2.08	0.51
1:C:162:LYS:NZ	2:C:401:N15:H13	2.26	0.51
1:G:188:LEU:HG	1:G:246:TYR:CE2	2.38	0.51
1:E:157:PHE:CE2	1:E:159:LEU:HD13	2.45	0.51
1:C:335:GLN:O	1:C:338:TYR:HB3	2.11	0.51
1:C:258:LYS:N	3:C:514:HOH:O	2.44	0.51
1:A:231:GLN:HA	1:A:386:ASN:O	2.11	0.51
1:C:225:LEU:O	1:C:227:LYS:N	2.35	0.51
1:C:273:ALA:O	1:C:274:ASP:HB2	2.10	0.51
1:A:257:ILE:HG21	1:A:314:SER:HB3	1.93	0.51
1:A:359:LEU:HD22	1:A:363:LEU:HD22	1.92	0.51
1:E:166:LYS:O	1:E:168:GLN:N	2.44	0.51
1:G:162:LYS:NZ	2:G:401:N15:H13	2.26	0.50
1:E:258:LYS:N	3:E:526:HOH:O	2.44	0.50
1:C:157:PHE:HE2	1:C:159:LEU:HD11	1.77	0.50
1:E:162:LYS:NZ	2:E:401:N15:H13	2.26	0.50
1:G:142:GLY:O	1:G:143:LYS:CG	2.47	0.50
1:E:301:ILE:HD12	1:E:338:TYR:CD1	2.47	0.50
1:E:366:HIS:O	1:E:368:PRO:HD3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:LEU:O	1:E:227:LYS:N	2.37	0.50
1:C:157:PHE:HE2	1:C:159:LEU:CD1	2.24	0.50
1:C:382:TRP:O	1:C:386:ASN:ND2	2.31	0.49
2:C:401:N15:H25	3:C:532:HOH:O	2.12	0.49
1:E:155:SER:O	1:E:156:LYS:HB2	2.11	0.49
2:E:401:N15:CAN	2:E:401:N15:O	2.60	0.49
1:C:166:LYS:O	1:C:168:GLN:O	2.30	0.49
1:A:141:LYS:NZ	1:C:326:LYS:NZ	2.61	0.49
1:E:194:LEU:HD21	2:E:401:N15:H17	1.93	0.49
1:C:194:LEU:HD23	2:C:401:N15:H16	1.94	0.49
1:C:200:PHE:CE1	1:C:209:ILE:HD11	2.48	0.49
1:G:382:TRP:CD1	1:G:386:ASN:ND2	2.80	0.49
1:A:229:ASP:O	1:A:233:THR:HG23	2.13	0.48
1:E:240:LEU:HD13	1:E:270:LEU:CD2	2.43	0.48
1:G:229:ASP:O	1:G:233:THR:HG22	2.13	0.48
1:A:382:TRP:O	1:A:386:ASN:OD1	2.32	0.48
1:A:141:LYS:HZ2	1:C:326:LYS:NZ	2.11	0.48
1:C:262:LEU:HD11	1:C:318:LEU:HD21	1.95	0.48
1:C:184:ILE:O	1:C:188:LEU:HG	2.13	0.48
1:A:317:VAL:HG13	1:A:328:PRO:HD2	1.95	0.48
1:E:140:GLY:O	1:E:141:LYS:C	2.53	0.47
1:G:140:GLY:C	1:G:142:GLY:N	2.67	0.47
1:E:231:GLN:HA	1:E:386:ASN:O	2.14	0.47
1:E:359:LEU:CD1	1:E:383:ILE:HD13	2.44	0.47
1:C:184:ILE:HD12	1:C:188:LEU:HD11	1.97	0.47
1:G:181:GLU:CG	1:G:182:VAL:HG23	2.35	0.47
1:A:221:GLU:HG3	1:A:264:LEU:CD1	2.44	0.47
1:C:193:ILE:HG12	1:C:272:ILE:HG12	1.97	0.47
1:G:131:GLU:CD	1:G:131:GLU:H	2.19	0.46
1:G:167:ALA:O	1:G:168:GLN:HB2	2.14	0.46
1:E:327:PRO:HB2	3:E:502:HOH:O	2.15	0.46
1:E:295:TYR:OH	1:E:321:GLU:OE1	2.30	0.46
2:E:401:N15:H8	2:E:401:N15:O	2.16	0.46
1:A:384:THR:O	1:A:385:ALA:HB3	2.16	0.46
1:G:344:VAL:HG12	1:G:346:PHE:CE2	2.51	0.46
1:E:340:ARG:HG3	1:E:340:ARG:HH11	1.80	0.46
1:A:182:VAL:HG23	1:A:196:LEU:HD21	1.98	0.46
1:G:182:VAL:HG13	1:G:196:LEU:HD21	1.98	0.46
1:A:184:ILE:HG13	1:A:185:GLN:N	2.30	0.46
2:E:401:N15:H25	3:E:515:HOH:O	2.16	0.46
1:C:168:GLN:HE21	1:C:168:GLN:HB2	1.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:TRP:O	1:C:386:ASN:HB2	2.15	0.45
1:G:240:LEU:CD1	1:G:272:ILE:HD11	2.46	0.45
1:E:157:PHE:CD2	1:E:159:LEU:HD13	2.51	0.45
1:A:383:ILE:HA	1:A:383:ILE:HD13	1.84	0.45
1:G:162:LYS:HZ3	2:G:401:N15:H13	1.81	0.45
1:C:134:GLU:O	1:C:150:ALA:HA	2.17	0.45
1:E:166:LYS:HE3	1:E:201:HIS:HB2	1.98	0.45
1:A:188:LEU:HG	1:A:246:TYR:HE2	1.81	0.45
1:E:190:HIS:ND1	1:E:191:PRO:HD2	2.31	0.45
1:E:327:PRO:HG2	1:E:330:GLU:HG3	1.99	0.44
1:G:185:GLN:HA	1:G:188:LEU:HB3	1.99	0.44
1:E:380:HIS:HD2	1:E:382:TRP:N	2.12	0.44
1:C:222:LEU:HD21	1:C:321:GLU:HG2	1.99	0.44
1:C:353:THR:O	1:C:357:ARG:HB2	2.17	0.44
1:A:262:LEU:HD13	1:A:270:LEU:HD11	1.98	0.44
1:E:321:GLU:HG3	1:E:326:LYS:C	2.37	0.44
2:C:401:N15:H8	2:C:401:N15:O	2.17	0.44
1:A:244:LEU:HD21	1:A:257:ILE:HD11	2.00	0.44
1:G:140:GLY:C	1:G:142:GLY:H	2.20	0.43
1:G:240:LEU:HG	1:G:315:LEU:CD1	2.48	0.43
1:A:257:ILE:O	1:A:257:ILE:HG22	2.18	0.43
1:E:359:LEU:HD22	1:E:363:LEU:CD2	2.47	0.43
1:C:231:GLN:HG3	1:C:386:ASN:O	2.18	0.43
1:C:194:LEU:HD21	2:C:401:N15:H17	1.99	0.43
1:G:162:LYS:CE	2:G:401:N15:O	2.66	0.43
1:G:194:LEU:HD23	2:G:401:N15:H16	1.99	0.43
1:E:261:ASN:HD21	1:E:274:ASP:HB2	1.84	0.43
1:G:199:TYR:OH	3:G:509:HOH:O	2.21	0.43
1:A:257:ILE:CG2	1:A:314:SER:HB3	2.48	0.43
1:G:327:PRO:HB2	3:G:510:HOH:O	2.19	0.42
1:A:143:LYS:HG2	1:C:332:ASN:HA	1.99	0.42
1:G:382:TRP:O	1:G:386:ASN:HB2	2.19	0.42
1:C:162:LYS:HB3	1:C:208:LEU:HB2	2.00	0.42
1:G:301:ILE:HD12	1:G:338:TYR:CD1	2.53	0.42
1:E:151:ARG:NH1	3:E:520:HOH:O	2.52	0.42
1:G:142:GLY:C	1:G:144:PHE:H	2.23	0.42
1:G:215:LEU:HA	1:G:215:LEU:HD23	1.90	0.42
1:C:383:ILE:HA	1:C:383:ILE:HD13	1.84	0.42
1:A:273:ALA:O	1:A:274:ASP:HB2	2.19	0.42
1:C:327:PRO:HB2	3:C:502:HOH:O	2.20	0.42
1:A:141:LYS:HB3	1:A:141:LYS:HE3	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLN:O	1:A:338:TYR:HB3	2.20	0.42
1:A:190:HIS:CE1	1:A:191:PRO:HD2	2.55	0.42
1:G:157:PHE:HD2	1:G:159:LEU:HD13	1.84	0.42
1:A:134:GLU:HB2	1:A:151:ARG:HB3	2.01	0.42
1:C:189:ARG:HH11	1:C:195:ARG:HD2	1.85	0.41
1:E:146:ASN:N	1:E:146:ASN:OD1	2.47	0.41
1:G:194:LEU:HD21	2:G:401:N15:H17	2.03	0.41
1:C:182:VAL:HG13	1:C:196:LEU:HD21	2.02	0.41
1:E:262:LEU:HB3	1:E:270:LEU:CD1	2.51	0.41
1:A:354:GLU:OE2	1:A:357:ARG:CD	2.66	0.41
1:A:231:GLN:O	1:A:235:THR:HG23	2.21	0.41
1:A:295:TYR:N	1:A:295:TYR:CD1	2.88	0.41
1:A:155:SER:O	1:A:156:LYS:HB2	2.19	0.41
1:A:297:PRO:HG3	1:A:310:VAL:HB	2.03	0.41
1:E:153:LYS:O	1:E:153:LYS:HD2	2.20	0.41
1:C:137:ARG:HG2	1:C:137:ARG:HH21	1.85	0.41
1:G:262:LEU:HB3	1:G:270:LEU:HD11	2.00	0.41
1:E:273:ALA:O	1:E:274:ASP:HB2	2.20	0.41
1:C:269:GLU:HG3	1:C:269:GLU:H	1.40	0.41
1:A:141:LYS:HZ1	1:C:326:LYS:HZ2	1.69	0.41
1:C:265:GLY:HA3	1:C:269:GLU:OE2	2.20	0.41
1:C:317:VAL:HG13	1:C:328:PRO:HD2	2.03	0.40
1:E:380:HIS:CD2	1:E:380:HIS:C	2.94	0.40
1:G:353:THR:O	1:G:357:ARG:HG3	2.21	0.40
1:G:221:GLU:HG3	1:G:264:LEU:HD11	2.04	0.40
1:E:382:TRP:CD1	1:E:386:ASN:ND2	2.89	0.40
1:C:199:TYR:HB2	1:C:208:LEU:HD23	2.03	0.40
1:E:162:LYS:NZ	2:E:401:N15:O	2.51	0.40
1:G:147:VAL:HA	1:G:161:LEU:O	2.21	0.40
1:A:321:GLU:HG3	1:A:326:LYS:C	2.42	0.40
1:G:137:ARG:HD3	3:G:501:HOH:O	2.21	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	189/261 (72%)	171 (90%)	14 (7%)	4 (2%)	9 6
1	C	188/261 (72%)	172 (92%)	12 (6%)	4 (2%)	9 6
1	E	188/261 (72%)	173 (92%)	11 (6%)	4 (2%)	9 6
1	G	188/261 (72%)	173 (92%)	12 (6%)	3 (2%)	12 11
All	All	753/1044 (72%)	689 (92%)	49 (6%)	15 (2%)	9 7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	LYS
1	A	387	SER
1	C	182	VAL
1	C	387	SER
1	E	167	ALA
1	G	141	LYS
1	A	226	SER
1	C	143	LYS
1	C	226	SER
1	E	141	LYS
1	G	224	LYS
1	G	294	ASP
1	A	294	ASP
1	E	142	GLY
1	E	226	SER

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	178/230 (77%)	153 (86%)	25 (14%)	4 3
1	C	175/230 (76%)	147 (84%)	28 (16%)	3 2
1	E	176/230 (76%)	150 (85%)	26 (15%)	4 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	176/230 (76%)	158 (90%)	18 (10%)	9 10
All	All	705/920 (77%)	608 (86%)	97 (14%)	4 4

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LYS
1	A	147	VAL
1	A	149	LEU
1	A	159	LEU
1	A	165	PHE
1	A	168	GLN
1	A	183	GLU
1	A	186	SER
1	A	191	PRO
1	A	199	TYR
1	A	225	LEU
1	A	229	ASP
1	A	233	THR
1	A	235	THR
1	A	238	THR
1	A	257	ILE
1	A	258	LYS
1	A	269	GLU
1	A	302	GLU
1	A	310	VAL
1	A	333	THR
1	A	359	LEU
1	A	362	ARG
1	A	363	LEU
1	A	383	ILE
1	C	147	VAL
1	C	159	LEU
1	C	161	LEU
1	C	165	PHE
1	C	168	GLN
1	C	183	GLU
1	C	189	ARG
1	C	199	TYR
1	C	204	THR
1	C	226	SER
1	C	227	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	229	ASP
1	C	232	ARG
1	C	233	THR
1	C	238	THR
1	C	240	LEU
1	C	244	LEU
1	C	269	GLU
1	C	292	THR
1	C	326	LYS
1	C	344	VAL
1	C	352	VAL
1	C	354	GLU
1	C	357	ARG
1	C	358	ASP
1	C	359	LEU
1	C	363	LEU
1	C	383	ILE
1	E	131	GLU
1	E	143	LYS
1	E	147	VAL
1	E	163	VAL
1	E	165	PHE
1	E	183	GLU
1	E	195	ARG
1	E	204	THR
1	E	225	LEU
1	E	226	SER
1	E	227	LYS
1	E	229	ASP
1	E	235	THR
1	E	238	THR
1	E	240	LEU
1	E	244	LEU
1	E	269	GLU
1	E	270	LEU
1	E	310	VAL
1	E	347	THR
1	E	350	ASP
1	E	354	GLU
1	E	359	LEU
1	E	362	ARG
1	E	363	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	383	ILE
1	G	147	VAL
1	G	163	VAL
1	G	165	PHE
1	G	184	ILE
1	G	199	TYR
1	G	204	THR
1	G	225	LEU
1	G	227	LYS
1	G	233	THR
1	G	238	THR
1	G	240	LEU
1	G	302	GLU
1	G	312	LEU
1	G	351	PHE
1	G	354	GLU
1	G	359	LEU
1	G	363	LEU
1	G	383	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	ASN
1	C	168	GLN
1	E	380	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	$\#\|Z\| > 2$
2	N15	A	401	-	32,36,36	3.63	15 (46%)	29,51,51	2.56	6 (20%)
2	N15	C	401	-	32,36,36	3.69	12 (37%)	29,51,51	2.90	7 (24%)
2	N15	E	401	-	32,36,36	3.53	13 (40%)	29,51,51	2.25	7 (24%)
2	N15	G	401	-	32,36,36	4.04	14 (43%)	29,51,51	2.05	7 (24%)

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
2	N15	A	401	-	-	0/13/18/18	0/5/5/5
2	N15	C	401	-	-	0/13/18/18	0/5/5/5
2	N15	E	401	-	-	0/13/18/18	0/5/5/5
2	N15	G	401	-	-	0/13/18/18	0/5/5/5

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	N15	NAP-N	-15.12	1.13	1.35
2	C	401	N15	NAP-N	-12.94	1.16	1.35
2	A	401	N15	NAT-NAQ	-11.64	1.14	1.37
2	E	401	N15	NAP-N	-10.61	1.20	1.35
2	E	401	N15	NAT-NAQ	-9.64	1.18	1.37
2	C	401	N15	NAT-NAQ	-9.52	1.18	1.37
2	G	401	N15	NAT-NAQ	-8.67	1.20	1.37
2	A	401	N15	CAZ-CAY	-7.92	1.34	1.49
2	A	401	N15	NAP-N	-7.86	1.24	1.35
2	G	401	N15	CAZ-CAY	-7.59	1.35	1.49
2	E	401	N15	CAZ-CAY	-7.41	1.35	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	N15	CAZ-CAY	-6.70	1.37	1.49
2	G	401	N15	CAK-CBC	-6.51	1.31	1.41
2	G	401	N15	CAX-CAW	-5.70	1.34	1.49
2	A	401	N15	CAX-CAW	-5.52	1.34	1.49
2	E	401	N15	CAK-CBC	-5.49	1.33	1.41
2	E	401	N15	CAX-CAW	-5.30	1.35	1.49
2	A	401	N15	CAK-CBC	-5.25	1.33	1.41
2	C	401	N15	CAX-CAW	-5.22	1.35	1.49
2	C	401	N15	CAK-CBC	-5.09	1.34	1.41
2	C	401	N15	CAH-CBB	-4.41	1.33	1.41
2	A	401	N15	CAH-CBB	-3.94	1.34	1.41
2	G	401	N15	CAG-CBA	-3.74	1.35	1.41
2	A	401	N15	CAG-CBA	-3.67	1.35	1.41
2	A	401	N15	CAI-CBD	-3.58	1.35	1.42
2	E	401	N15	CAH-CBB	-3.52	1.35	1.41
2	A	401	N15	CBD-CBC	-3.51	1.33	1.42
2	E	401	N15	CAI-CBD	-3.50	1.35	1.42
2	C	401	N15	CAI-CBD	-3.47	1.35	1.42
2	G	401	N15	CAI-CBD	-3.26	1.35	1.42
2	C	401	N15	CBD-CBC	-3.14	1.34	1.42
2	G	401	N15	CAH-CBB	-3.11	1.36	1.41
2	A	401	N15	CA-N	-2.97	1.43	1.47
2	G	401	N15	CBD-CBC	-2.72	1.35	1.42
2	G	401	N15	CAL-CAX	-2.52	1.34	1.38
2	E	401	N15	CAL-CAX	-2.50	1.34	1.38
2	C	401	N15	CAG-CBA	-2.50	1.37	1.41
2	A	401	N15	CBA-CBB	-2.49	1.34	1.42
2	E	401	N15	CAG-CBA	-2.39	1.37	1.41
2	C	401	N15	CBA-CBB	-2.36	1.34	1.42
2	E	401	N15	CBD-CBC	-2.34	1.36	1.42
2	A	401	N15	CAY-NAR	-2.28	1.32	1.35
2	G	401	N15	CAY-NAR	-2.27	1.32	1.35
2	G	401	N15	CBA-CBB	-2.22	1.34	1.42
2	G	401	N15	CA-N	-2.16	1.44	1.47
2	A	401	N15	CAL-CAX	-2.09	1.34	1.38
2	E	401	N15	CBA-CBB	-2.09	1.35	1.42
2	C	401	N15	CAL-CAX	-2.02	1.35	1.38
2	E	401	N15	CA-N	-2.00	1.44	1.47
2	A	401	N15	CAI-CAF	2.20	1.41	1.36
2	C	401	N15	CAE-CAH	2.31	1.42	1.36
2	A	401	N15	CAE-CAH	2.48	1.42	1.36
2	G	401	N15	CAE-CAH	2.69	1.42	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	N15	CAE-CAH	2.93	1.43	1.36

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	N15	CAJ-CAX-CAW	-7.87	117.82	127.84
2	A	401	N15	CAJ-CAX-CAW	-6.91	119.04	127.84
2	E	401	N15	CAJ-CAX-CAW	-6.29	119.83	127.84
2	G	401	N15	CAJ-CAX-CAW	-5.51	120.83	127.84
2	A	401	N15	C-CA-N	-4.36	105.02	110.68
2	E	401	N15	CAM-NAS-C	-2.74	117.41	122.79
2	C	401	N15	CAM-NAS-C	-2.66	117.55	122.79
2	C	401	N15	CAE-CAD-CAG	-2.41	116.94	120.45
2	E	401	N15	CAD-CAE-CAH	-2.39	116.97	120.45
2	A	401	N15	CAI-CAF-CAW	-2.36	117.04	121.14
2	G	401	N15	CAI-CAF-CAW	-2.31	117.13	121.14
2	G	401	N15	CAK-CAW-CAX	-2.16	117.00	121.16
2	E	401	N15	CAL-N-NAP	2.25	113.53	111.56
2	C	401	N15	C-CA-N	2.34	113.72	110.68
2	G	401	N15	CAL-N-NAP	2.62	113.85	111.56
2	G	401	N15	CAL-CAX-CAW	2.65	131.21	127.84
2	G	401	N15	CA-N-CAL	3.14	133.20	129.19
2	E	401	N15	CAL-CAX-CAW	3.24	131.96	127.84
2	A	401	N15	CAJ-NAP-N	3.72	108.10	104.24
2	A	401	N15	CAL-CAX-CAW	3.89	132.79	127.84
2	E	401	N15	CAJ-NAP-N	4.18	108.57	104.24
2	C	401	N15	CAL-CAX-CAW	5.25	134.51	127.84
2	C	401	N15	CAJ-NAP-N	6.01	110.47	104.24
2	G	401	N15	CAJ-NAP-N	6.19	110.65	104.24
2	E	401	N15	CA-N-CAL	6.21	137.11	129.19
2	A	401	N15	CA-N-CAL	8.32	139.79	129.19
2	C	401	N15	CA-N-CAL	8.92	140.57	129.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	N15	4	0
2	C	401	N15	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	N15	7	0
2	G	401	N15	5	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^{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	203/261 (77%)	1.09	31 (15%)	3 2	28, 47, 67, 84	0
1	C	202/261 (77%)	1.11	28 (13%)	4 3	30, 47, 68, 79	0
1	E	202/261 (77%)	1.07	31 (15%)	3 2	30, 47, 69, 78	0
1	G	202/261 (77%)	1.29	42 (20%)	1 1	31, 47, 69, 76	0
All	All	809/1044 (77%)	1.14	132 (16%)	2 2	28, 47, 69, 84	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	273	ALA	11.0
1	G	274	ASP	6.9
1	E	247	CYS	6.0
1	G	293	LEU	5.6
1	G	387	SER	5.6
1	C	385	ALA	5.5
1	C	300	MET	5.4
1	G	364	LEU	5.2
1	G	367	ASN	5.2
1	G	128	TRP	5.1
1	E	218	VAL	4.9
1	C	273	ALA	4.9
1	G	383	ILE	4.8
1	C	187	HIS	4.7
1	G	182	VAL	4.4
1	E	238	THR	4.4
1	E	182	VAL	4.4
1	A	332	ASN	4.4
1	C	219	TYR	4.2
1	G	331	ALA	4.1
1	E	367	ASN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	367	ASN	4.0
1	G	300	MET	3.9
1	C	184	ILE	3.9
1	C	311	ASP	3.8
1	A	199	TYR	3.7
1	C	293	LEU	3.7
1	C	380	HIS	3.7
1	A	222	LEU	3.7
1	G	243	ALA	3.7
1	E	222	LEU	3.7
1	G	247	CYS	3.6
1	G	366	HIS	3.6
1	C	350	ASP	3.6
1	E	334	TYR	3.6
1	C	140	GLY	3.5
1	A	209	ILE	3.5
1	C	387	SER	3.5
1	G	313	TRP	3.4
1	G	181	GLU	3.4
1	G	222	LEU	3.3
1	A	269	GLU	3.3
1	C	144	PHE	3.3
1	A	146	ASN	3.2
1	E	232	ARG	3.2
1	E	354	GLU	3.2
1	A	334	TYR	3.2
1	G	333	THR	3.1
1	G	302	GLU	3.1
1	E	141	LYS	3.1
1	C	182	VAL	3.0
1	E	193	ILE	3.0
1	G	229	ASP	3.0
1	A	318	LEU	3.0
1	G	155	SER	2.9
1	E	302	GLU	2.9
1	G	368	PRO	2.9
1	C	267	ALA	2.9
1	C	270	LEU	2.8
1	A	272	ILE	2.8
1	E	144	PHE	2.8
1	C	272	ILE	2.8
1	A	363	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	313	TRP	2.7
1	E	206	VAL	2.7
1	E	383	ILE	2.7
1	A	302	GLU	2.7
1	A	273	ALA	2.7
1	G	359	LEU	2.7
1	A	166	LYS	2.7
1	G	186	SER	2.7
1	G	149	LEU	2.6
1	E	188	LEU	2.6
1	A	201	HIS	2.6
1	C	216	GLY	2.6
1	G	198	GLY	2.6
1	G	386	ASN	2.6
1	A	300	MET	2.6
1	E	201	HIS	2.5
1	A	220	ARG	2.5
1	E	196	LEU	2.5
1	A	316	GLY	2.5
1	E	220	ARG	2.4
1	G	363	LEU	2.4
1	A	187	HIS	2.4
1	E	163	VAL	2.4
1	C	147	VAL	2.4
1	A	186	SER	2.4
1	C	384	THR	2.3
1	E	350	ASP	2.3
1	E	264	LEU	2.3
1	G	240	LEU	2.3
1	G	183	GLU	2.3
1	A	184	ILE	2.2
1	G	267	ALA	2.2
1	A	159	LEU	2.2
1	C	310	VAL	2.2
1	C	203	ALA	2.2
1	G	343	ARG	2.2
1	C	292	THR	2.2
1	C	368	PRO	2.2
1	E	332	ASN	2.2
1	A	381	PRO	2.2
1	A	340	ARG	2.2
1	E	266	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	333	THR	2.2
1	G	147	VAL	2.2
1	E	199	TYR	2.2
1	G	385	ALA	2.2
1	G	295	TYR	2.1
1	G	321	GLU	2.1
1	E	381	PRO	2.1
1	C	324	VAL	2.1
1	G	325	GLY	2.1
1	G	167	ALA	2.1
1	G	211	GLU	2.1
1	G	207	TYR	2.1
1	A	233	THR	2.1
1	E	342	SER	2.1
1	C	221	GLU	2.1
1	E	310	VAL	2.1
1	A	384	THR	2.1
1	A	141	LYS	2.1
1	C	246	TYR	2.0
1	A	185	GLN	2.0
1	A	196	LEU	2.0
1	A	328	PRO	2.0
1	G	199	TYR	2.0
1	G	329	PHE	2.0
1	A	367	ASN	2.0
1	A	229	ASP	2.0
1	E	293	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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^{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	LLDF	B-factors(Å^2)	Q<0.9
2	N15	A	401	32/32	0.91	0.22	-0.01	27,36,54,57	0
2	N15	G	401	32/32	0.84	0.19	-0.50	30,34,53,56	0
2	N15	E	401	32/32	0.89	0.20	-0.69	28,34,52,55	0
2	N15	C	401	32/32	0.93	0.17	-0.94	26,33,54,55	0

6.5 Other polymers (i)

There are no such residues in this entry.