



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:59 AM UTC

PDB ID : 2PQJ / pdb_00002pqj
Title : Crystal structure of active ribosome inactivating protein from maize (b-32), complex with adenine
Authors : Mak, A.N.S.; Au, S.W.N.; Cha, S.S.; Young, J.A.; Wong, K.B.; Shaw, P.C.
Deposited on : 2007-05-02
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

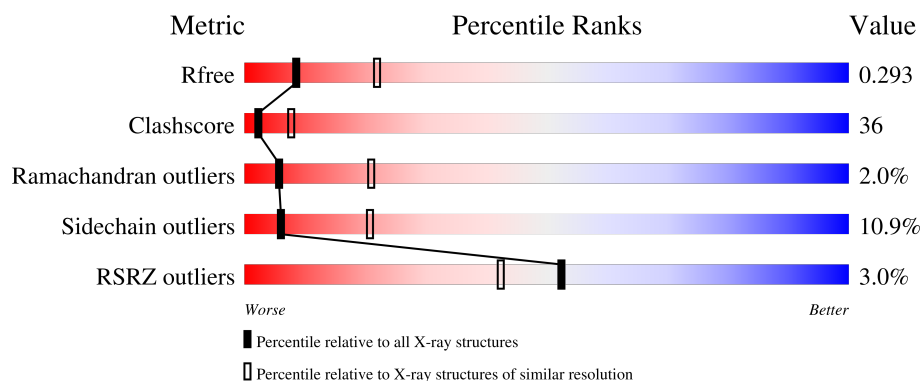
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	243	2% 42% 43% 9% • •
1	B	243	44% 44% 7% 5%
1	C	243	6% 43% 42% 10% • 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADE	B	501	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5427 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.

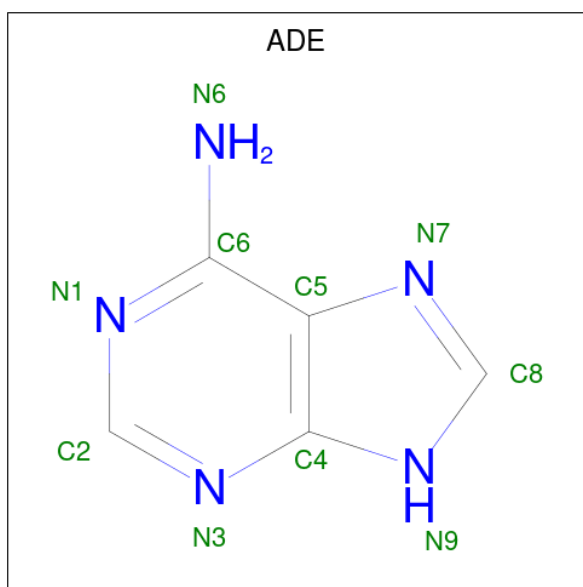
- Molecule 1 is a protein called Ribosome-inactivating protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1800	1153	313	326	8			
1	B	232	Total	C	N	O	S	0	0	0
			1786	1144	306	328	8			
1	C	232	Total	C	N	O	S	0	0	0
			1796	1151	312	326	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	expression tag	UNP P25891
A	165	LEU	-	linker	UNP P25891
A	166	GLU	-	linker	UNP P25891
B	21	MET	-	expression tag	UNP P25891
B	165	LEU	-	linker	UNP P25891
B	166	GLU	-	linker	UNP P25891
C	21	MET	-	expression tag	UNP P25891
C	165	LEU	-	linker	UNP P25891
C	166	GLU	-	linker	UNP P25891

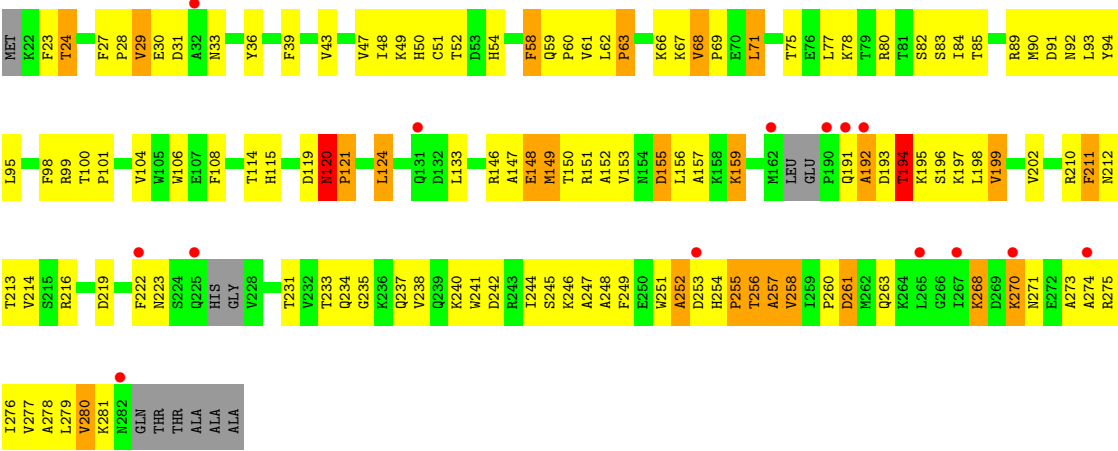
- Molecule 2 is ADENINE (CCD ID: ADE) (formula: C₅H₅N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	5	5		
2	B	1	Total	C	N	0	0
			10	5	5		
2	C	1	Total	C	N	0	0
			10	5	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	6	Total	O	0	0
			6	6		
3	C	3	Total	O	0	0
			3	3		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	115.91Å 115.91Å 44.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.99 – 2.80 40.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.99-2.80) 99.9 (40.99-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.293 0.238 , 0.293	Depositor DCC
R_{free} test set	843 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 73.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l 0.025 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5427	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.57	0/1840	1.06	12/2495 (0.5%)
1	B	0.56	0/1826	1.05	12/2480 (0.5%)
1	C	0.48	0/1834	0.98	8/2484 (0.3%)
All	All	0.54	0/5500	1.03	32/7459 (0.4%)

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	3
1	C	0	2
All	All	0	5

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	VAL	N-CA-C	7.11	117.25	110.42
1	C	252	ALA	N-CA-C	-6.72	104.30	113.30
1	C	124	LEU	N-CA-C	-6.65	105.13	113.18
1	A	36	TYR	N-CA-C	-6.54	104.24	111.82
1	B	194	THR	N-CA-C	-6.51	105.16	113.23
1	B	212	ASN	N-CA-C	-6.34	104.45	111.36
1	B	252	ALA	N-CA-C	-6.32	104.48	111.82
1	B	195	LYS	N-CA-C	-6.26	104.54	111.36
1	A	248	ALA	N-CA-C	-6.26	104.54	111.36
1	A	205	VAL	N-CA-C	6.25	116.43	110.74
1	B	193	ASP	N-CA-C	-6.09	105.50	113.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	THR	N-CA-C	-5.98	105.94	113.18
1	A	157	ALA	N-CA-C	-5.92	105.89	113.23
1	C	58	PHE	N-CA-C	5.76	118.30	111.33
1	A	206	CYS	N-CA-C	5.71	117.18	111.07
1	C	211	PHE	N-CA-C	5.62	117.89	108.73
1	B	102	GLY	N-CA-C	-5.51	106.14	115.34
1	B	273	ALA	N-CA-C	-5.50	105.19	111.14
1	A	59	GLN	N-CA-C	5.42	118.15	110.24
1	B	257	ALA	N-CA-C	5.33	117.40	110.53
1	C	193	ASP	N-CA-C	-5.29	106.60	113.16
1	A	82	SER	N-CA-C	5.28	116.03	108.74
1	B	256	THR	N-CA-C	5.17	118.74	112.23
1	A	150	THR	N-CA-C	-5.16	105.11	111.40
1	A	282	ASN	N-CA-C	5.15	115.97	108.14
1	B	94	TYR	N-CA-C	5.15	117.64	109.24
1	B	127	GLY	N-CA-C	5.11	119.10	112.25
1	A	268	LYS	N-CA-C	5.04	116.58	111.14
1	C	261	ASP	N-CA-C	-5.04	105.68	111.07
1	C	29	VAL	N-CA-C	5.01	115.23	110.42
1	A	62	LEU	CA-C-N	5.00	123.31	119.66
1	A	62	LEU	C-N-CA	5.00	123.31	119.66

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	LEU	Peptide
1	A	281	LYS	Peptide
1	A	282	ASN	Peptide
1	C	120	ASN	Peptide
1	C	192	ALA	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	1800	0	1781	124	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1786	0	1753	129	0
1	C	1796	0	1783	142	0
2	A	10	0	4	2	0
2	B	10	0	4	5	0
2	C	10	0	4	2	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	3	0	0	0	0
All	All	5427	0	5329	387	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 36.

All (387) 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:59:GLN:HE21	1:A:277:VAL:CG2	1.53	1.21
1:C:152:ALA:HA	1:C:197:LYS:HD2	1.28	1.11
1:C:211:PHE:HB3	1:C:213:THR:HG22	1.37	1.05
1:A:59:GLN:NE2	1:A:277:VAL:CG2	2.24	1.01
1:C:231:THR:H	1:C:234:GLN:HE21	1.12	0.97
1:B:264:LYS:HG3	1:C:254:HIS:CE1	1.99	0.97
1:B:118:GLY:O	1:B:121:PRO:HD3	1.65	0.96
1:A:106:TRP:HZ2	1:A:160:LYS:O	1.49	0.94
1:B:37:SER:HB3	1:B:219:ASP:OD1	1.68	0.94
1:C:212:ASN:O	1:C:216:ARG:HG2	1.69	0.93
1:B:231:THR:H	1:B:234:GLN:HE21	1.10	0.92
1:A:26:ILE:HG21	1:A:78:LYS:HD3	1.53	0.91
1:B:50:HIS:HB2	1:B:90:MET:HE1	1.51	0.89
1:C:268:LYS:HE2	1:C:268:LYS:N	1.87	0.89
1:A:106:TRP:NE1	1:A:159:LYS:HG2	1.86	0.89
1:B:50:HIS:CB	1:B:90:MET:HE1	2.04	0.88
1:A:152:ALA:HA	1:A:197:LYS:HD2	1.57	0.87
1:C:50:HIS:HB2	1:C:90:MET:HE1	1.57	0.87
1:B:264:LYS:HG3	1:C:254:HIS:NE2	1.88	0.86
1:C:192:ALA:HB1	1:C:195:LYS:HG3	1.55	0.85
1:A:59:GLN:HE21	1:A:277:VAL:HG23	1.37	0.85
1:A:211:PHE:HB3	1:A:213:THR:HG22	1.59	0.85
1:A:106:TRP:CZ2	1:A:160:LYS:O	2.30	0.85
1:B:127:GLY:HA3	1:B:132:ASP:OD2	1.79	0.83
1:B:258:VAL:HG12	1:B:263:GLN:OE1	1.79	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:HIS:HD2	1:B:257:ALA:HB2	1.43	0.82
1:C:29:VAL:HG13	1:C:149:MET:HG2	1.62	0.81
1:A:59:GLN:HE21	1:A:277:VAL:HG22	1.43	0.81
1:B:37:SER:CB	1:B:219:ASP:OD1	2.31	0.79
1:C:231:THR:H	1:C:234:GLN:NE2	1.80	0.79
1:C:24:THR:HG22	1:C:75:THR:HA	1.63	0.78
1:A:50:HIS:HB2	1:A:90:MET:HE1	1.66	0.78
1:B:211:PHE:HB3	1:B:213:THR:HG22	1.64	0.78
1:A:268:LYS:HE2	1:A:268:LYS:N	2.00	0.77
1:A:59:GLN:HB3	1:A:278:ALA:O	1.84	0.77
1:A:250:GLU:CD	1:A:259:ILE:HD13	2.09	0.77
1:A:250:GLU:CD	1:A:259:ILE:CD1	2.59	0.76
1:C:268:LYS:HE2	1:C:268:LYS:H	1.48	0.75
1:A:106:TRP:HE1	1:A:159:LYS:HG2	1.51	0.75
1:B:24:THR:HB	1:B:75:THR:HG22	1.69	0.75
1:C:52:THR:OG1	1:C:54:HIS:HE1	1.69	0.74
1:A:115:HIS:CE1	1:A:123:TRP:NE1	2.55	0.74
1:C:59:GLN:NE2	1:C:277:VAL:HG23	2.01	0.74
1:A:79:THR:HG21	1:A:154:ASN:HD21	1.50	0.74
1:B:268:LYS:N	1:B:268:LYS:HE2	2.02	0.74
1:B:59:GLN:HB3	1:B:278:ALA:O	1.88	0.74
1:A:59:GLN:HB2	1:A:280:VAL:HG13	1.68	0.73
1:B:192:ALA:HB1	1:B:195:LYS:HG3	1.71	0.73
1:C:51:CYS:SG	1:C:62:LEU:HD23	2.28	0.73
1:B:264:LYS:HE3	1:C:254:HIS:CE1	2.24	0.72
1:B:231:THR:H	1:B:234:GLN:NE2	1.86	0.72
1:B:107:GLU:HB2	1:B:117:LEU:HD12	1.72	0.72
1:C:256:THR:O	1:C:257:ALA:O	2.08	0.71
1:B:264:LYS:CG	1:C:254:HIS:CE1	2.71	0.71
1:C:211:PHE:HB2	1:C:214:VAL:HG23	1.70	0.71
1:C:39:PHE:O	1:C:43:VAL:HG23	1.91	0.71
1:B:240:LYS:HG3	1:B:265:LEU:HD11	1.73	0.71
1:B:24:THR:HG22	1:B:75:THR:HA	1.72	0.70
1:C:115:HIS:CD2	1:C:121:PRO:HB2	2.27	0.70
1:B:251:TRP:CH2	1:B:262:MET:HG3	2.26	0.70
1:C:62:LEU:HD21	1:C:279:LEU:HD13	1.73	0.70
1:C:77:LEU:HD22	1:C:149:MET:HE1	1.73	0.70
1:C:119:ASP:O	1:C:120:ASN:CG	2.34	0.70
1:C:194:THR:O	1:C:198:LEU:HG	1.91	0.70
1:B:26:ILE:HG22	1:B:27:PHE:N	2.06	0.70
1:C:133:LEU:HD12	1:C:199:VAL:HG23	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:THR:OG1	1:B:43:VAL:HG22	1.92	0.69
1:B:83:SER:O	1:B:101:PRO:HG3	1.91	0.69
1:A:231:THR:H	1:A:234:GLN:NE2	1.90	0.68
1:C:77:LEU:HD13	1:C:149:MET:HE3	1.74	0.68
1:B:254:HIS:CD2	1:B:256:THR:OG1	2.46	0.67
1:C:69:PRO:HD3	1:C:89:ARG:NH2	2.09	0.67
1:C:58:PHE:HD2	1:C:274:ALA:CB	2.08	0.67
1:B:259:ILE:O	1:B:262:MET:N	2.27	0.67
1:A:79:THR:HG21	1:A:154:ASN:ND2	2.10	0.66
1:C:254:HIS:O	1:C:256:THR:N	2.28	0.66
1:C:28:PRO:HB2	1:C:31:ASP:HB3	1.79	0.65
1:A:231:THR:H	1:A:234:GLN:HE21	1.44	0.65
1:B:21:MET:HE2	1:B:72:TRP:CD1	2.32	0.65
1:B:35:PRO:HG2	1:B:38:ALA:HB2	1.79	0.65
1:C:119:ASP:O	1:C:120:ASN:CB	2.44	0.64
1:A:107:GLU:HG2	1:A:123:TRP:CZ3	2.33	0.64
1:A:149:MET:HB2	1:A:204:MET:HE1	1.79	0.63
1:C:59:GLN:HB3	1:C:278:ALA:O	1.98	0.63
1:B:130:TYR:CD1	1:B:139:LEU:HD11	2.34	0.63
1:C:71:LEU:HD12	1:C:90:MET:SD	2.38	0.63
1:A:106:TRP:CE3	1:A:122:ARG:O	2.52	0.63
1:B:24:THR:HG21	1:B:75:THR:HB	1.81	0.63
1:A:26:ILE:HG21	1:A:78:LYS:CD	2.27	0.62
1:A:59:GLN:NE2	1:A:277:VAL:HG21	2.12	0.62
1:C:31:ASP:OD1	1:C:33:ASN:HB2	1.99	0.62
1:B:37:SER:N	1:B:219:ASP:OD1	2.33	0.61
1:B:254:HIS:CD2	1:B:257:ALA:HB2	2.32	0.61
1:B:50:HIS:HB2	1:B:90:MET:CE	2.27	0.61
1:A:24:THR:HB	1:A:75:THR:HA	1.83	0.60
1:C:52:THR:OG1	1:C:54:HIS:CE1	2.53	0.60
1:B:152:ALA:HA	1:B:197:LYS:HD2	1.83	0.60
1:B:24:THR:CB	1:B:75:THR:HG22	2.31	0.60
1:B:192:ALA:CB	1:B:195:LYS:HG3	2.31	0.60
1:C:59:GLN:HE21	1:C:277:VAL:HG23	1.66	0.60
1:B:272:GLU:O	1:B:275:ARG:HB2	2.01	0.59
1:B:264:LYS:CE	1:C:254:HIS:HE1	2.15	0.59
1:B:207:GLU:HA	1:B:207:GLU:OE1	2.02	0.59
1:C:147:ALA:O	1:C:150:THR:HB	2.02	0.59
1:C:231:THR:N	1:C:234:GLN:HE21	1.92	0.59
1:A:94:TYR:HA	2:A:501:ADE:C2	2.37	0.59
1:C:77:LEU:HD22	1:C:149:MET:CE	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:PHE:CD2	1:C:274:ALA:CB	2.85	0.59
1:A:58:PHE:CD1	1:A:270:LYS:HE2	2.38	0.59
1:C:24:THR:HG21	1:C:75:THR:HB	1.85	0.59
1:C:68:VAL:HG12	1:C:68:VAL:O	2.03	0.59
1:A:115:HIS:CE1	1:A:123:TRP:CE2	2.91	0.58
1:B:24:THR:CG2	1:B:75:THR:HA	2.34	0.58
1:B:130:TYR:CE2	2:B:501:ADE:C6	2.91	0.58
1:A:79:THR:CG2	1:A:154:ASN:HD21	2.15	0.58
1:B:115:HIS:CD2	1:B:121:PRO:HG2	2.39	0.58
1:C:253:ASP:C	1:C:254:HIS:HD1	2.11	0.58
1:B:30:GLU:OE2	1:B:79:THR:HB	2.04	0.58
1:B:251:TRP:CE3	1:B:270:LYS:HA	2.39	0.57
1:A:101:PRO:CD	1:A:157:ALA:HB1	2.34	0.57
1:B:254:HIS:O	1:B:256:THR:N	2.37	0.57
1:C:85:THR:O	1:C:98:PHE:HA	2.04	0.57
1:C:260:PRO:HA	1:C:263:GLN:CG	2.34	0.57
1:A:82:SER:OG	1:A:83:SER:N	2.36	0.57
1:B:138:GLY:O	1:B:141:THR:HG23	2.05	0.57
1:C:94:TYR:HA	2:C:501:ADE:C2	2.39	0.57
1:B:264:LYS:HE3	1:C:254:HIS:HE1	1.69	0.56
1:C:24:THR:CG2	1:C:75:THR:HA	2.34	0.56
1:B:35:PRO:HG2	1:B:38:ALA:CB	2.35	0.56
1:B:207:GLU:OE2	2:B:501:ADE:C2	2.58	0.56
1:C:90:MET:O	1:C:91:ASP:C	2.48	0.56
1:A:92:ASN:HB3	1:A:281:LYS:HE2	1.87	0.56
1:B:231:THR:N	1:B:234:GLN:HE21	1.91	0.56
1:A:106:TRP:HB3	1:A:124:LEU:HG	1.87	0.56
1:A:59:GLN:NE2	1:A:277:VAL:HG22	2.11	0.55
1:A:131:GLN:HA	1:A:135:GLY:HA2	1.88	0.55
1:A:260:PRO:O	1:A:264:LYS:HG2	2.06	0.55
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.71	0.55
1:C:151:ARG:O	1:C:155:ASP:HB2	2.07	0.55
1:C:50:HIS:CB	1:C:90:MET:HE1	2.33	0.55
1:B:59:GLN:HB2	1:B:280:VAL:HG23	1.89	0.55
1:C:47:VAL:HA	1:C:90:MET:HE3	1.89	0.55
1:C:231:THR:HG23	1:C:234:GLN:NE2	2.22	0.55
1:C:58:PHE:HD2	1:C:274:ALA:HB1	1.72	0.55
1:B:254:HIS:C	1:B:256:THR:H	2.15	0.55
1:B:258:VAL:CG1	1:B:263:GLN:OE1	2.53	0.55
1:C:152:ALA:CA	1:C:197:LYS:HD2	2.18	0.55
1:C:69:PRO:HD3	1:C:89:ARG:HH22	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:MET:HB2	1:A:204:MET:CE	2.37	0.54
1:B:26:ILE:CG2	1:B:27:PHE:N	2.68	0.54
1:C:95:LEU:N	2:C:501:ADE:N1	2.52	0.54
1:A:58:PHE:CE1	1:A:270:LYS:HE2	2.43	0.54
1:C:50:HIS:HB2	1:C:90:MET:CE	2.36	0.54
1:C:258:VAL:O	1:C:260:PRO:HD3	2.08	0.54
1:B:211:PHE:CZ	1:B:238:VAL:HA	2.43	0.54
1:A:47:VAL:HG13	1:A:90:MET:HE3	1.88	0.54
1:C:92:ASN:HB3	1:C:281:LYS:HE2	1.91	0.53
1:C:84:ILE:HG12	1:C:153:VAL:HG13	1.91	0.53
1:C:192:ALA:HB1	1:C:195:LYS:CG	2.36	0.53
1:A:119:ASP:O	1:A:120:ASN:C	2.52	0.53
1:A:44:ARG:O	1:A:48:ILE:HG13	2.08	0.52
1:B:127:GLY:HA3	1:B:132:ASP:CG	2.34	0.52
1:B:24:THR:HG21	1:B:75:THR:CB	2.39	0.52
1:A:31:ASP:OD2	1:A:34:TYR:CE2	2.62	0.52
1:A:26:ILE:HG22	1:A:27:PHE:N	2.24	0.52
1:A:241:TRP:CH2	1:A:281:LYS:HG3	2.45	0.52
1:C:149:MET:O	1:C:153:VAL:HG23	2.09	0.52
1:B:110:LYS:O	1:B:113:ASP:HB2	2.10	0.52
1:B:234:GLN:O	1:B:238:VAL:HG23	2.10	0.52
1:B:271:ASN:O	1:B:274:ALA:HB3	2.10	0.52
1:C:60:PRO:HD2	1:C:279:LEU:HD23	1.92	0.52
1:C:279:LEU:C	1:C:280:VAL:CG1	2.82	0.52
1:C:29:VAL:HG22	1:C:149:MET:HE2	1.92	0.51
1:C:273:ALA:O	1:C:277:VAL:HG22	2.09	0.51
1:C:36:TYR:O	1:C:39:PHE:HB3	2.10	0.51
1:C:211:PHE:HB2	1:C:214:VAL:CG2	2.38	0.51
1:A:250:GLU:CD	1:A:259:ILE:HD11	2.36	0.51
1:B:231:THR:HG23	1:B:234:GLN:NE2	2.25	0.51
1:A:122:ARG:O	1:A:123:TRP:C	2.53	0.51
1:B:264:LYS:CE	1:C:254:HIS:CE1	2.92	0.51
1:C:149:MET:O	1:C:149:MET:HG3	2.10	0.51
1:A:250:GLU:OE2	1:A:259:ILE:HD13	2.09	0.51
1:B:78:LYS:HB2	1:B:83:SER:HB3	1.92	0.51
1:C:198:LEU:O	1:C:202:VAL:HG23	2.11	0.51
1:A:211:PHE:CZ	1:A:238:VAL:HA	2.45	0.51
1:A:48:ILE:C	1:A:50:HIS:N	2.65	0.51
1:C:242:ASP:O	1:C:246:LYS:HG3	2.10	0.50
1:B:63:PRO:HG2	1:B:90:MET:HE2	1.92	0.50
1:B:144:MET:HB2	1:B:228:VAL:HG13	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:O	1:A:43:VAL:HG23	2.11	0.50
1:A:280:VAL:HG23	1:A:281:LYS:N	2.26	0.50
1:A:119:ASP:O	1:A:120:ASN:O	2.30	0.50
1:B:130:TYR:CE1	1:B:139:LEU:HD11	2.46	0.50
1:C:48:ILE:C	1:C:50:HIS:N	2.66	0.50
1:B:59:GLN:HG2	1:B:277:VAL:O	2.12	0.50
1:A:48:ILE:C	1:A:50:HIS:H	2.19	0.50
1:A:99:ARG:CZ	1:A:103:GLY:HA2	2.42	0.50
1:A:144:MET:O	1:A:228:VAL:HG12	2.12	0.50
1:C:80:ARG:HG2	1:C:80:ARG:HH11	1.76	0.50
1:A:85:THR:HB	1:A:99:ARG:HB3	1.94	0.49
1:C:43:VAL:O	1:C:47:VAL:HG23	2.12	0.49
1:C:95:LEU:HG	1:C:108:PHE:HE1	1.76	0.49
1:B:251:TRP:CG	1:B:270:LYS:HB3	2.47	0.49
1:C:254:HIS:N	1:C:255:PRO:HD3	2.26	0.49
1:B:24:THR:HG23	1:B:25:GLU:O	2.12	0.49
1:B:202:VAL:O	1:B:206:CYS:HB2	2.12	0.49
1:A:256:THR:O	1:A:257:ALA:C	2.56	0.49
1:B:129:ARG:O	1:B:132:ASP:N	2.37	0.49
1:B:264:LYS:CG	1:C:254:HIS:HE1	2.24	0.49
1:C:61:VAL:HG11	1:C:249:PHE:HZ	1.77	0.49
1:C:279:LEU:C	1:C:280:VAL:HG12	2.38	0.49
1:B:259:ILE:O	1:B:261:ASP:N	2.46	0.49
1:A:251:TRP:CE3	1:A:270:LYS:HA	2.48	0.48
1:B:280:VAL:HG12	1:B:281:LYS:N	2.28	0.48
1:B:242:ASP:O	1:B:242:ASP:OD2	2.31	0.48
1:A:154:ASN:N	1:A:154:ASN:HD22	2.10	0.48
1:B:254:HIS:C	1:B:256:THR:N	2.69	0.48
1:A:151:ARG:O	1:A:155:ASP:HB2	2.14	0.48
1:A:260:PRO:HA	1:A:263:GLN:HB2	1.95	0.48
1:C:194:THR:O	1:C:198:LEU:CG	2.58	0.48
1:C:254:HIS:C	1:C:256:THR:N	2.72	0.48
1:A:30:GLU:OE2	1:A:80:ARG:HG2	2.13	0.48
1:A:83:SER:O	1:A:101:PRO:HG3	2.14	0.48
1:B:48:ILE:HA	1:B:51:CYS:SG	2.54	0.48
1:A:29:VAL:O	1:A:146:ARG:NH2	2.43	0.48
1:C:66:LYS:O	1:C:67:LYS:C	2.57	0.48
1:C:191:GLN:O	1:C:191:GLN:HG3	2.13	0.48
1:A:225:GLN:OE1	1:A:226:HIS:CE1	2.66	0.48
1:B:36:TYR:O	1:B:39:PHE:HB3	2.13	0.48
1:C:36:TYR:HD2	1:C:219:ASP:HB2	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ARG:O	1:C:278:ALA:HB3	2.12	0.48
1:C:233:THR:O	1:C:237:GLN:HG3	2.14	0.48
1:B:211:PHE:HB2	1:B:214:VAL:HG23	1.94	0.47
1:C:156:LEU:O	1:C:159:LYS:HB3	2.14	0.47
1:C:211:PHE:CZ	1:C:238:VAL:HA	2.49	0.47
1:C:245:SER:O	1:C:248:ALA:HB3	2.14	0.47
1:A:126:PHE:CD2	1:A:195:LYS:HE2	2.48	0.47
1:C:66:LYS:O	1:C:68:VAL:N	2.47	0.47
1:C:85:THR:HB	1:C:99:ARG:HB3	1.96	0.47
1:B:99:ARG:HB2	1:B:105:TRP:CE2	2.50	0.47
1:C:260:PRO:HA	1:C:263:GLN:HG3	1.94	0.47
1:A:69:PRO:HG2	1:A:72:TRP:CZ2	2.49	0.47
1:B:251:TRP:HB3	1:B:270:LYS:HB3	1.96	0.47
1:A:93:LEU:HD11	1:A:279:LEU:HD13	1.96	0.46
1:B:126:PHE:CG	1:B:195:LYS:HE2	2.50	0.46
1:C:237:GLN:HE22	1:C:276:ILE:CD1	2.28	0.46
1:B:203:VAL:HA	1:B:207:GLU:HG2	1.96	0.46
1:B:254:HIS:NE2	1:B:256:THR:OG1	2.43	0.46
1:C:237:GLN:NE2	1:C:276:ILE:HD13	2.29	0.46
1:B:93:LEU:HD11	1:B:279:LEU:HD12	1.97	0.46
1:B:210:ARG:O	1:B:278:ALA:N	2.45	0.46
1:B:196:SER:O	1:B:200:LYS:HG3	2.15	0.46
1:A:107:GLU:OE1	1:A:115:HIS:HD2	1.99	0.46
1:C:82:SER:OG	1:C:101:PRO:HG2	2.16	0.46
1:B:36:TYR:HD2	1:B:219:ASP:HB2	1.81	0.46
1:B:262:MET:HB3	1:B:267:ILE:HB	1.98	0.46
1:C:100:THR:OG1	1:C:104:VAL:HB	2.15	0.46
1:A:117:LEU:HD23	1:A:117:LEU:N	2.30	0.46
1:C:242:ASP:OD1	1:C:246:LYS:HE3	2.15	0.46
1:A:24:THR:HG22	1:A:25:GLU:O	2.16	0.46
1:A:30:GLU:HG2	1:A:150:THR:HG21	1.97	0.46
1:A:43:VAL:HB	1:A:209:LEU:HD21	1.98	0.46
1:A:106:TRP:HE3	1:A:122:ARG:O	1.97	0.46
1:A:126:PHE:CG	1:A:195:LYS:HE2	2.51	0.46
1:B:273:ALA:C	1:B:275:ARG:N	2.73	0.46
1:A:95:LEU:HB3	2:A:501:ADE:H61	1.81	0.45
1:A:135:GLY:C	1:A:137:LYS:H	2.24	0.45
1:A:264:LYS:HA	1:A:264:LYS:HD3	1.77	0.45
1:A:48:ILE:O	1:A:50:HIS:N	2.50	0.45
1:A:59:GLN:NE2	1:A:277:VAL:HG23	2.13	0.45
1:B:260:PRO:HA	1:B:263:GLN:HG3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:THR:HG21	1:C:75:THR:CB	2.46	0.45
1:C:78:LYS:HB2	1:C:83:SER:HB3	1.97	0.45
1:A:272:GLU:O	1:A:275:ARG:HG2	2.16	0.45
1:B:130:TYR:HE2	2:B:501:ADE:N1	2.14	0.45
1:C:254:HIS:C	1:C:256:THR:H	2.25	0.45
1:A:30:GLU:CD	1:A:80:ARG:HG2	2.41	0.45
1:A:138:GLY:CA	1:A:140:GLU:OE1	2.65	0.45
1:B:59:GLN:OE1	1:B:59:GLN:N	2.47	0.45
1:A:24:THR:HG21	1:A:75:THR:HB	1.98	0.45
1:A:259:ILE:O	1:A:262:MET:N	2.49	0.45
1:A:87:ALA:HB2	1:A:105:TRP:CZ3	2.52	0.45
1:A:101:PRO:HD3	1:A:157:ALA:HB1	1.99	0.45
1:C:29:VAL:CG1	1:C:149:MET:HG2	2.38	0.45
1:A:120:ASN:N	1:A:121:PRO:HD3	2.31	0.45
1:A:267:ILE:C	1:A:268:LYS:HE2	2.41	0.45
1:C:92:ASN:O	1:C:93:LEU:C	2.61	0.45
1:A:259:ILE:HA	1:A:260:PRO:HD2	1.71	0.44
1:A:216:ARG:HA	1:A:216:ARG:HD3	1.65	0.44
1:C:119:ASP:O	1:C:120:ASN:HB2	2.15	0.44
1:C:251:TRP:CE3	1:C:270:LYS:HA	2.52	0.44
1:A:250:GLU:OE1	1:A:259:ILE:HD13	2.17	0.44
1:C:62:LEU:O	1:C:63:PRO:C	2.59	0.44
1:A:138:GLY:HA3	1:A:140:GLU:OE1	2.16	0.44
1:A:268:LYS:HD2	1:A:272:GLU:OE1	2.18	0.44
1:C:68:VAL:O	1:C:69:PRO:C	2.61	0.44
1:A:109:GLY:HA3	1:A:123:TRP:CE3	2.53	0.44
1:A:233:THR:O	1:A:237:GLN:HG3	2.18	0.44
1:B:259:ILE:O	1:B:260:PRO:C	2.60	0.44
1:C:71:LEU:HB3	1:C:90:MET:HB2	2.00	0.44
1:B:62:LEU:O	1:B:63:PRO:C	2.61	0.44
1:A:106:TRP:CZ3	1:A:122:ARG:O	2.71	0.44
1:A:244:ILE:HA	1:A:262:MET:SD	2.58	0.44
1:A:93:LEU:HD11	1:A:279:LEU:CD1	2.47	0.44
1:A:108:PHE:O	1:A:123:TRP:HZ3	2.01	0.44
1:A:212:ASN:O	1:A:216:ARG:HG2	2.18	0.44
1:B:129:ARG:HA	2:B:501:ADE:H62	1.82	0.44
1:B:280:VAL:CG1	1:B:281:LYS:N	2.81	0.44
1:C:119:ASP:O	1:C:120:ASN:OD1	2.35	0.44
1:B:50:HIS:CG	1:B:90:MET:HE1	2.51	0.43
1:B:37:SER:CA	1:B:219:ASP:OD1	2.66	0.43
1:B:39:PHE:O	1:B:43:VAL:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:O	1:A:206:CYS:HB2	2.18	0.43
1:B:44:ARG:O	1:B:48:ILE:HG13	2.18	0.43
1:A:231:THR:O	1:A:232:VAL:C	2.61	0.43
1:B:260:PRO:HA	1:B:263:GLN:CG	2.49	0.43
1:B:134:ILE:O	1:B:137:LYS:HB2	2.19	0.43
1:C:244:ILE:O	1:C:247:ALA:HB3	2.19	0.43
1:A:230:LEU:HB3	1:A:234:GLN:HE21	1.82	0.43
1:B:34:TYR:HD1	1:B:34:TYR:C	2.27	0.43
1:B:85:THR:O	1:B:98:PHE:HA	2.18	0.43
1:B:273:ALA:O	1:B:274:ALA:C	2.61	0.43
1:C:29:VAL:HG12	1:C:150:THR:OG1	2.19	0.43
1:C:30:GLU:CD	1:C:80:ARG:HG3	2.44	0.43
1:C:211:PHE:CB	1:C:214:VAL:HG23	2.42	0.43
1:C:106:TRP:HB3	1:C:124:LEU:HG	2.01	0.43
1:C:254:HIS:O	1:C:255:PRO:C	2.61	0.43
1:B:140:GLU:H	1:B:140:GLU:CD	2.27	0.42
1:C:133:LEU:CD1	1:C:199:VAL:HG23	2.46	0.42
1:C:146:ARG:HB2	1:C:222:PHE:CD1	2.54	0.42
1:C:254:HIS:N	1:C:255:PRO:CD	2.82	0.42
1:B:63:PRO:HG2	1:B:71:LEU:HD12	2.01	0.42
1:B:130:TYR:OH	1:B:202:VAL:HG12	2.20	0.42
1:B:40:ILE:O	1:B:44:ARG:HG3	2.18	0.42
1:C:106:TRP:NE1	1:C:159:LYS:HG2	2.34	0.42
1:B:34:TYR:C	1:B:34:TYR:CD1	2.97	0.42
1:B:45:LYS:O	1:B:49:LYS:HG3	2.19	0.42
1:C:78:LYS:CB	1:C:83:SER:HB3	2.49	0.42
1:A:143:THR:HA	1:A:229:THR:HG22	2.01	0.42
1:A:206:CYS:O	1:A:210:ARG:HG3	2.20	0.42
1:C:146:ARG:HB2	1:C:222:PHE:CE1	2.54	0.42
1:C:237:GLN:HE22	1:C:276:ILE:HD13	1.84	0.42
1:C:27:PHE:HE1	1:C:149:MET:SD	2.43	0.42
1:C:58:PHE:CD2	1:C:274:ALA:HB2	2.55	0.42
1:A:138:GLY:O	1:A:140:GLU:N	2.52	0.42
1:B:238:VAL:C	1:B:240:LYS:H	2.26	0.42
1:B:120:ASN:H	1:B:120:ASN:HD22	1.67	0.42
1:B:251:TRP:CB	1:B:270:LYS:HB3	2.50	0.42
1:C:120:ASN:HA	1:C:121:PRO:HD3	1.38	0.42
1:A:259:ILE:O	1:A:261:ASP:N	2.54	0.41
1:B:77:LEU:HD11	1:B:86:LEU:HD11	2.02	0.41
1:C:242:ASP:OD2	1:C:281:LYS:HD3	2.21	0.41
1:A:65:GLU:C	1:A:66:LYS:HG3	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:C	1:A:134:ILE:HG23	2.45	0.41
1:B:21:MET:N	1:B:72:TRP:H	2.18	0.41
1:B:259:ILE:CG2	1:B:262:MET:HG2	2.50	0.41
1:C:157:ALA:C	1:C:159:LYS:H	2.27	0.41
1:C:240:LYS:O	1:C:241:TRP:C	2.63	0.41
1:C:234:GLN:O	1:C:235:GLY:C	2.63	0.41
1:B:120:ASN:HD22	1:B:120:ASN:N	2.17	0.41
1:B:225:GLN:C	1:B:227:GLY:H	2.28	0.41
1:C:234:GLN:O	1:C:237:GLN:HB2	2.21	0.41
1:A:138:GLY:O	1:A:140:GLU:OE1	2.39	0.41
1:A:258:VAL:HG13	1:A:263:GLN:OE1	2.21	0.41
1:B:115:HIS:CE1	1:B:123:TRP:NE1	2.88	0.41
1:A:138:GLY:C	1:A:140:GLU:OE1	2.64	0.41
1:B:86:LEU:HB3	1:B:95:LEU:HD11	2.03	0.41
1:C:48:ILE:O	1:C:49:LYS:C	2.64	0.41
1:A:29:VAL:O	1:A:146:ARG:HG3	2.21	0.41
1:A:124:LEU:HD22	1:A:126:PHE:CZ	2.56	0.41
1:B:130:TYR:CE2	2:B:501:ADE:N1	2.89	0.41
1:B:146:ARG:HB2	1:B:222:PHE:CD1	2.56	0.41
1:B:269:ASP:OD1	1:B:271:ASN:HB2	2.21	0.41
1:C:48:ILE:C	1:C:50:HIS:H	2.28	0.41
1:C:148:GLU:C	1:C:150:THR:N	2.78	0.41
1:A:107:GLU:HG2	1:A:123:TRP:HZ3	1.85	0.40
1:A:207:GLU:OE1	1:A:210:ARG:HD2	2.22	0.40
1:C:82:SER:O	1:C:83:SER:HB3	2.20	0.40
1:C:197:LYS:HA	1:C:197:LYS:HD3	1.78	0.40
1:B:211:PHE:CZ	1:B:241:TRP:HB2	2.56	0.40
1:C:256:THR:O	1:C:257:ALA:C	2.64	0.40
1:A:31:ASP:OD2	1:A:34:TYR:CD2	2.75	0.40
1:A:38:ALA:O	1:A:39:PHE:C	2.64	0.40
1:A:250:GLU:OE2	1:A:259:ILE:CD1	2.68	0.40
1:C:252:ALA:C	1:C:253:ASP:OD2	2.64	0.40
1:A:30:GLU:CG	1:A:150:THR:HG21	2.52	0.40
1:C:192:ALA:HA	1:C:194:THR:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/243 (94%)	198 (86%)	25 (11%)	6 (3%)	4	15
1	B	228/243 (94%)	201 (88%)	24 (10%)	3 (1%)	9	31
1	C	226/243 (93%)	181 (80%)	40 (18%)	5 (2%)	5	19
All	All	683/729 (94%)	580 (85%)	89 (13%)	14 (2%)	6	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ASP
1	C	120	ASN
1	C	257	ALA
1	A	139	LEU
1	C	255	PRO
1	A	121	PRO
1	C	121	PRO
1	A	260	PRO
1	B	221	GLY
1	A	120	ASN
1	B	255	PRO
1	A	134	ILE
1	B	276	ILE
1	C	63	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/206 (91%)	163 (87%)	24 (13%)	4	15
1	B	186/206 (90%)	170 (91%)	16 (9%)	10	31
1	C	187/206 (91%)	166 (89%)	21 (11%)	6	19
All	All	560/618 (91%)	499 (89%)	61 (11%)	6	21

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	75	THR
1	A	81	THR
1	A	110	LYS
1	A	124	LEU
1	A	129	ARG
1	A	134	ILE
1	A	137	LYS
1	A	140	GLU
1	A	143	THR
1	A	155	ASP
1	A	193	ASP
1	A	194	THR
1	A	199	VAL
1	A	242	ASP
1	A	254	HIS
1	A	256	THR
1	A	259	ILE
1	A	268	LYS
1	A	270	LYS
1	A	277	VAL
1	A	280	VAL
1	A	281	LYS
1	A	283	GLN
1	B	24	THR
1	B	25	GLU
1	B	26	ILE
1	B	57	ILE
1	B	78	LYS
1	B	82	SER
1	B	92	ASN
1	B	194	THR
1	B	258	VAL
1	B	268	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	269	ASP
1	B	270	LYS
1	B	275	ARG
1	B	276	ILE
1	B	277	VAL
1	B	281	LYS
1	C	23	PHE
1	C	24	THR
1	C	68	VAL
1	C	71	LEU
1	C	114	THR
1	C	148	GLU
1	C	149	MET
1	C	155	ASP
1	C	159	LYS
1	C	194	THR
1	C	196	SER
1	C	199	VAL
1	C	223	ASN
1	C	256	THR
1	C	258	VAL
1	C	261	ASP
1	C	268	LYS
1	C	270	LYS
1	C	271	ASN
1	C	275	ARG
1	C	280	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	92	ASN
1	A	115	HIS
1	A	154	ASN
1	A	225	GLN
1	A	226	HIS
1	A	234	GLN
1	B	54	HIS
1	B	115	HIS
1	B	120	ASN
1	B	154	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	234	GLN
1	B	237	GLN
1	B	254	HIS
1	C	54	HIS
1	C	92	ASN
1	C	154	ASN
1	C	234	GLN
1	C	263	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	ADE	C	501	-	11,11,11	1.13	0	15,15,15	2.74	6 (40%)
2	ADE	B	501	-	11,11,11	1.27	1 (9%)	15,15,15	2.75	6 (40%)
2	ADE	A	501	-	11,11,11	1.09	0	15,15,15	2.82	6 (40%)

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	ADE	C	501	-	-	-	0/2/2/2
2	ADE	B	501	-	-	-	0/2/2/2
2	ADE	A	501	-	-	-	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ADE	C5-C4	2.68	1.43	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ADE	C5-N7-C8	5.51	109.70	103.48
2	C	501	ADE	C5-N7-C8	5.36	109.53	103.48
2	B	501	ADE	C5-N7-C8	5.36	109.53	103.48
2	B	501	ADE	N9-C4-N3	5.18	135.08	126.69
2	A	501	ADE	N9-C4-N3	5.11	134.97	126.69
2	C	501	ADE	N9-C4-N3	5.07	134.90	126.69
2	A	501	ADE	N3-C2-N1	-4.39	121.94	128.58
2	B	501	ADE	C5-C4-N3	-4.17	119.14	126.75
2	C	501	ADE	N3-C2-N1	-4.09	122.39	128.58
2	C	501	ADE	C5-C4-N3	-4.08	119.31	126.75
2	A	501	ADE	C5-C4-N3	-4.06	119.36	126.75
2	B	501	ADE	N3-C2-N1	-4.03	122.48	128.58
2	B	501	ADE	C4-C5-N7	-2.77	106.82	110.67
2	C	501	ADE	C4-C5-N7	-2.72	106.89	110.67
2	A	501	ADE	C4-C5-N7	-2.72	106.90	110.67
2	A	501	ADE	N9-C8-N7	-2.52	110.03	113.87
2	C	501	ADE	N9-C8-N7	-2.37	110.26	113.87
2	B	501	ADE	N9-C8-N7	-2.29	110.39	113.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	ADE	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	ADE	5	0
2	A	501	ADE	2	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, 95th 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	233/243 (95%)	0.00	6 (2%) 57 47	20, 55, 79, 101	0
1	B	232/243 (95%)	-0.04	1 (0%) 88 84	28, 55, 77, 90	0
1	C	232/243 (95%)	0.67	14 (6%) 27 21	37, 76, 100, 126	0
All	All	697/729 (95%)	0.21	21 (3%) 52 42	20, 60, 94, 126	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	GLY	4.5
1	C	267	ILE	3.1
1	A	192	ALA	2.9
1	C	282	ASN	2.8
1	C	225	GLN	2.7
1	C	162	MET	2.7
1	A	119	ASP	2.6
1	C	192	ALA	2.6
1	C	265	LEU	2.6
1	A	282	ASN	2.5
1	C	274	ALA	2.4
1	C	191	GLN	2.3
1	C	222	PHE	2.2
1	C	270	LYS	2.2
1	B	131	GLN	2.2
1	C	32	ALA	2.2
1	C	253	ASP	2.2
1	A	135	GLY	2.1
1	A	22	LYS	2.1
1	C	190	PRO	2.1
1	C	131	GLN	2.1

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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($\text{\AA}^2$)	Q<0.9
2	ADE	B	501	10/10	0.56	0.25	90,101,103,104	0
2	ADE	A	501	10/10	0.83	0.20	116,117,117,118	0
2	ADE	C	501	10/10	0.87	0.17	116,117,118,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.