

Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2023 – 02:18 PM EDT

PDB ID	:	1TYQ
Title	:	Crystal structure of $Arp2/3$ complex with bound ATP and calcium
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Deposited on	:	2004-07-08
Resolution	:	2.55 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
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: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.55 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.



Motria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	$1284 \ (2.56-2.52)$
Clashscore	141614	$1332 \ (2.56-2.52)$
Ramachandran outliers	138981	$1315 \ (2.56-2.52)$
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272(2.56-2.52)

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	А	418	5%	23%	• 5%
	D	204	7%	2370	- 570
2	В	394	32% 20% ·	47%	
3	С	372	64%	26%	• 8%
4	D	300	69%	21%	• 9%
5	Е	178	10%	32%	• 5%



Mol	Chain	Length	Quality of chai	n	
6	F	168	^{2%} 66%	29%	• •
7	G	151	62%	26%	• 11%



$1 \mathrm{TYQ}$

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13586 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 Actin-related protein 3.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	А	399	Total 3166	C 2031	N 527	O 594	S 14	0	0	0

• Molecule 2 is a protein called Actin-related Protein 2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	208	Total 1558	C 998	N 267	O 289	$\frac{S}{4}$	0	0	0

• Molecule 3 is a protein called Arp2/3 complex 41kDa subunit.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
3	С	342	Total 2641	C 1674	N 464	0 484	S 19	0	0	0

• Molecule 4 is a protein called Arp2/3 complex 34kDa subunit.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
4	D	274	Total 2219	C 1411	N 386	0 414	S 8	0	0	0

• Molecule 5 is a protein called Arp2/3 complex 21kDa subunit.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
5	Е	169	Total 1379	C 888	N 229	O 253	S 9	0	0	0

• Molecule 6 is a protein called Arp2/3 complex 20kDa subunit.



Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
6	F	166	Total 1364	C 871	N 238	O 246	S 9	0	0	0

• Molecule 7 is a protein called Arp2/3 Complex 16kDa Subunit.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	G	134	Total 1014	$\begin{array}{c} \mathrm{C} \\ 637 \end{array}$	N 174	O 200	${ m S} { m 3}$	0	0	0

• Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	Total Ca 1 1	0	0
8	В	1	Total Ca 1 1	0	0

• Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
0	Λ	1	Total	С	Ν	Ο	Р	0	0
9 A	1	31	10	5	13	3	0	0	
0	В	1	Total	С	Ν	Ο	Р	0	0
9 Б	1	31	10	5	13	3	0	U	

• Molecule 10 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	22	$\begin{array}{cc} \text{Total} & \text{O} \\ 22 & 22 \end{array}$	0	0
10	В	13	Total O 13 13	0	0
10	С	59	Total O 59 59	0	0
10	D	41	Total O 41 41	0	0
10	Е	2	Total O 2 2	0	0
10	F	37	Total O 37 37	0	0
10	G	7	Total O 7 7	0	0



3 Residue-property plots (i)

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



• Molecule 1: Actin-related protein 3



 • Molecule 7: Arp
2/3 Complex 16k Da Subunit







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	111.37Å 129.39Å 199.69Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	30.00 - 2.55	Depositor
Resolution (A)	29.60 - 2.57	EDS
% Data completeness	(Not available) $(30.00-2.55)$	Depositor
(in resolution range)	78.4 (29.60-2.57)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	$3.58 (at 2.57 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
B B.	0.232 , 0.272	Depositor
n, n_{free}	0.223 , 0.262	DCC
R_{free} test set	3662 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	50.3	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.37, 48.6	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13586	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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).

Mal	Chain	Bond lengths		Bond angles	
WIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.38	0/3247	0.59	0/4411
2	В	0.35	0/1586	0.59	0/2157
3	С	0.39	0/2708	0.66	1/3675~(0.0%)
4	D	0.38	0/2267	0.59	0/3058
5	Ε	0.34	0/1411	0.59	1/1900~(0.1%)
6	F	0.41	0/1386	0.62	0/1858
7	G	0.34	0/1026	0.55	0/1382
All	All	0.38	0/13631	0.60	2/18441~(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
4	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
5	Ε	17	GLY	N-CA-C	-5.88	98.41	113.10
3	С	11	ILE	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	261	TYR	Sidechain



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	А	3166	0	3062	79	0
2	В	1558	0	1506	67	0
3	С	2641	0	2597	81	0
4	D	2219	0	2180	56	0
5	Е	1379	0	1387	46	0
6	F	1364	0	1403	41	0
7	G	1014	0	1021	29	0
8	А	1	0	0	0	0
8	В	1	0	0	0	0
9	А	31	0	12	4	0
9	В	31	0	12	4	0
10	А	22	0	0	2	0
10	В	13	0	0	0	0
10	С	59	0	0	1	0
10	D	41	0	0	1	0
10	Ε	2	0	0	0	0
10	F	37	0	0	3	0
10	G	7	0	0	0	0
All	All	13586	0	13180	384	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
6:F:130:LYS:HA	6:F:130:LYS:HE2	1.40	1.00
4:D:170:LYS:HE2	4:D:170:LYS:HA	1.44	0.99
3:C:223:ASP:HB3	7:G:146:THR:HG21	1.43	0.99
3:C:216:ARG:HG2	3:C:230:ASP:HB3	1.47	0.97
2:B:205:ASN:HD22	2:B:208:ALA:H	1.13	0.97
1:A:191:LYS:HE2	1:A:303:VAL:HG22	1.45	0.96
6:F:4:THR:HG23	6:F:55:ARG:HE	1.29	0.95
3:C:371:ILE:HG22	3:C:372:VAL:HG23	1.50	0.94
1:A:257:THR:HG22	1:A:268:SER:HB3	1.50	0.93



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:C:183:THR:HG22	3:C:185:TRP:H	1.33	0.91
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.53	0.89
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.54	0.87
2:B:326:LEU:HD12	2:B:337:LEU:HD12	1.57	0.87
3:C:370:LYS:HD2	3:C:370:LYS:O	1.79	0.83
2:B:302:VAL:HG22	2:B:350:ARG:HH22	1.45	0.81
1:A:309:ILE:HD13	1:A:312:ARG:CZ	2.11	0.80
6:F:37:GLU:H	6:F:68:ASN:HD21	1.30	0.80
2:B:194:ILE:HG12	2:B:213:VAL:HG21	1.63	0.80
3:C:14:HIS:H	3:C:331:GLN:HE22	1.29	0.79
3:C:223:ASP:CB	7:G:146:THR:HG21	2.14	0.77
1:A:248:ASP:O	1:A:250:SER:N	2.18	0.76
2:B:314:PRO:O	2:B:318:GLU:HG3	1.86	0.75
2:B:205:ASN:HD22	2:B:208:ALA:N	1.84	0.74
7:G:62:PRO:CG	7:G:105:LEU:HD21	2.17	0.74
2:B:349:ARG:O	2:B:350:ARG:HB2	1.87	0.72
2:B:239:VAL:HG23	2:B:240:LEU:HD13	1.72	0.72
3:C:183:THR:HG22	3:C:185:TRP:N	2.05	0.71
2:B:157:VAL:HB	2:B:303:LEU:HD13	1.71	0.71
6:F:130:LYS:HA	6:F:130:LYS:CE	2.21	0.71
5:E:48:TYR:HB3	5:E:52:ASN:ND2	2.07	0.70
2:B:304:SER:HB3	2:B:350:ARG:NH1	2.07	0.69
7:G:62:PRO:HG2	7:G:105:LEU:HD21	1.73	0.69
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.75	0.68
5:E:9:MET:CE	5:E:13:THR:HB	2.23	0.68
3:C:321:LEU:N	3:C:321:LEU:HD12	2.09	0.68
5:E:123:LYS:O	5:E:127:GLU:HG3	1.93	0.68
3:C:155:VAL:HG21	3:C:180:PRO:CG	2.24	0.68
2:B:166:ILE:O	2:B:168:PRO:HD3	1.94	0.68
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.76	0.68
5:E:88:LYS:O	5:E:92:GLU:HG3	1.94	0.68
3:C:107:ASN:C	3:C:107:ASN:HD22	1.97	0.67
3:C:21:THR:HG22	3:C:22:GLN:HG3	1.77	0.67
3:C:107:ASN:ND2	3:C:109:LYS:H	1.92	0.67
3:C:119:VAL:HG23	3:C:137:ILE:O	1.94	0.67
7:G:87:LYS:HZ3	7:G:87:LYS:HB2	1.59	0.66
1:A:289:ASN:C	1:A:289:ASN:HD22	1.99	0.66
4:D:203:ARG:NH1	4:D:218:ASP:HA	2.11	0.66
6:F:101:PHE:O	6:F:103:ILE:N	2.28	0.66
1:A:194:PRO:O	1:A:195:ILE:HD12	1.96	0.66
5:E:62:ASN:C	5:E:62:ASN:HD22	1.99	0.65



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.77	0.65
4:D:203:ARG:NH2	4:D:218:ASP:OD1	2.27	0.65
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.78	0.65
3:C:229:ALA:HB2	3:C:237:VAL:HG22	1.78	0.65
1:A:91:ARG:O	1:A:94:GLU:HB2	1.97	0.64
6:F:4:THR:CG2	6:F:55:ARG:HE	2.08	0.64
7:G:95:VAL:HG21	7:G:131:LYS:HB3	1.80	0.64
2:B:282:LEU:HD21	2:B:301:ILE:HD13	1.81	0.63
1:A:243:ASN:ND2	5:E:47:TYR:HE1	1.96	0.63
4:D:129:PHE:HD2	4:D:237:ARG:HG3	1.65	0.62
2:B:218:GLU:HG2	9:B:1002:ATP:C5	2.34	0.62
2:B:219:LYS:HG2	2:B:220:LEU:HD13	1.80	0.62
3:C:193:GLU:HG3	3:C:195:MET:CE	2.30	0.62
5:E:62:ASN:ND2	5:E:65:ASP:H	1.98	0.62
2:B:184:ILE:HD12	2:B:185:ALA:N	2.14	0.61
5:E:130:ARG:HG3	5:E:130:ARG:HH11	1.65	0.61
3:C:14:HIS:H	3:C:331:GLN:NE2	1.98	0.61
2:B:345:GLU:C	2:B:347:PRO:HD3	2.21	0.61
4:D:137:GLU:CD	4:D:158:LYS:HE2	2.21	0.61
6:F:127:TYR:HB3	6:F:129:HIS:CE1	2.36	0.61
1:A:230:ARG:HH11	1:A:230:ARG:CB	2.14	0.61
1:A:246:ASP:OD1	5:E:50:LYS:HE3	2.01	0.61
4:D:228:PHE:H	4:D:231:HIS:HD2	1.49	0.61
6:F:145:GLU:O	6:F:149:MET:HG3	2.01	0.60
7:G:86:PHE:C	7:G:87:LYS:HD3	2.22	0.60
1:A:120:PRO:HB2	1:A:409:ARG:HG2	1.83	0.60
2:B:180:ARG:CB	2:B:281:LEU:HD21	2.31	0.60
6:F:20:LEU:HD23	6:F:70:VAL:HG21	1.84	0.60
1:A:229:GLU:HG2	9:A:1001:ATP:C5	2.36	0.60
3:C:167:ARG:HG2	3:C:197:GLU:HG3	1.83	0.60
6:F:137:HIS:CE1	6:F:141:GLU:HG3	2.37	0.60
2:B:163:VAL:HG22	2:B:164:THR:N	2.17	0.60
3:C:193:GLU:HG3	3:C:195:MET:HE1	1.83	0.60
6:F:80:ASP:OD1	6:F:82:ILE:HG22	2.02	0.60
3:C:119:VAL:HG22	3:C:120:ILE:N	2.17	0.59
6:F:68:ASN:C	6:F:68:ASN:HD22	2.06	0.59
6:F:121:PHE:O	6:F:125:GLN:HG2	2.02	0.59
1:A:384:LEU:HB3	1:A:414:PHE:CE1	2.36	0.59
2:B:205:ASN:ND2	2:B:208:ALA:H	1.92	0.59
7:G:62:PRO:HG3	7:G:105:LEU:HD21	1.84	0.59
2:B:151:LEU:HD13	2:B:300:HIS:HD2	1.68	0.58



	A L C	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:155:VAL:HG21	2:B:286:ILE:HD11	1.84	0.58	
7:G:87:LYS:HD3	7:G:87:LYS:N	2.19	0.58	
1:A:230:ARG:HH11	1:A:230:ARG:HB3	1.69	0.57	
2:B:326:LEU:HD12	2:B:337:LEU:CD1	2.31	0.57	
2:B:205:ASN:HB3	2:B:208:ALA:HB3	1.86	0.57	
2:B:182:LEU:HD22	2:B:184:ILE:HG23	1.86	0.57	
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.40	0.57	
3:C:29:ASN:HB3	3:C:31:GLU:H	1.69	0.57	
1:A:176:HIS:HD2	1:A:192:HIS:ND1	2.02	0.57	
2:B:184:ILE:CD1	2:B:188:ASP:HB2	2.35	0.57	
3:C:107:ASN:HD22	3:C:108:GLU:N	2.02	0.56	
4:D:95:LEU:HD11	4:D:116:LEU:HG	1.87	0.56	
3:C:143:SER:OG	3:C:162:CYS:HB2	2.05	0.56	
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.88	0.56	
4:D:223:ILE:HD12	4:D:223:ILE:N	2.21	0.56	
7:G:62:PRO:HG2	7:G:105:LEU:CD2	2.36	0.56	
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.40	0.56	
3:C:184:PRO:HB2	3:C:231:ALA:CB	2.35	0.56	
1:A:111:LEU:HD23	1:A:111:LEU:C	2.26	0.56	
1:A:374:ARG:NH1	9:A:1001:ATP:H8	2.02	0.56	
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.41	0.56	
1:A:339:LEU:O	1:A:343:VAL:HG12	2.06	0.56	
2:B:156:VAL:HG22	2:B:302:VAL:HG12	1.88	0.56	
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.41	0.55	
4:D:121:PHE:O	4:D:124:VAL:HG12	2.06	0.55	
7:G:44:SER:O	7:G:47:ARG:HG2	2.06	0.55	
5:E:16:ILE:HG23	5:E:16:ILE:O	2.07	0.55	
1:A:36:ALA:HB1	1:A:72:TYR:HB3	1.88	0.54	
7:G:47:ARG:HG3	7:G:48:GLN:HG3	1.90	0.54	
5:E:56:LYS:HA	5:E:169:MET:HA	1.89	0.54	
3:C:72:THR:HA	3:C:98:ALA:HB1	1.90	0.54	
3:C:183:THR:CG2	3:C:185:TRP:H	2.12	0.54	
6:F:95:MET:SD	6:F:108:PRO:HD3	2.48	0.54	
1:A:191:LYS:HB2	1:A:303:VAL:HG22	1.89	0.53	
5:E:78:CYS:O	5:E:82:LEU:HB2	2.09	0.53	
4:D:106:LYS:O	4:D:109:ILE:HG12	2.08	0.53	
2:B:310:TYR:CE1	9:B:1002:ATP:H2	2.26	0.53	
5:E:112:PRO:HG3	5:E:172:SER:O	2.08	0.53	
1:A:289:ASN:HD22	1:A:290:PRO:N	2.05	0.53	
1:A:30:ILE:HG12	1:A:375:TYR:CZ	2.43	0.53	
1:A:395:HIS:HB3	1:A:407:ILE:HD12	1.90	0.53	



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:B:302:VAL:HG22	2:B:350:ARG:NH2	2.20	0.53	
4:D:137:GLU:OE2	4:D:158:LYS:HE2	2.09	0.53	
4:D:171:ASP:OD2	4:D:172:ASP:N	2.42	0.53	
1:A:189:CYS:O	1:A:303:VAL:HG13	2.09	0.53	
4:D:71:GLY:HA2	4:D:74:GLU:OE1	2.09	0.53	
3:C:135:LYS:HB3	3:C:191:PHE:CZ	2.43	0.53	
1:A:106:GLU:HG2	1:A:135:ASN:HB3	1.90	0.52	
4:D:203:ARG:NH1	4:D:218:ASP:OD1	2.43	0.52	
1:A:81:GLY:O	1:A:115:PRO:HG2	2.09	0.52	
1:A:393:VAL:HG21	1:A:414:PHE:CD2	2.44	0.52	
4:D:37:ASP:HB2	4:D:43:TYR:HE1	1.73	0.52	
4:D:106:LYS:O	4:D:109:ILE:N	2.41	0.52	
1:A:176:HIS:CD2	1:A:192:HIS:ND1	2.78	0.52	
4:D:247:PHE:O	4:D:250:TYR:HB3	2.08	0.52	
1:A:311:VAL:C	1:A:314:PRO:HD2	2.30	0.52	
7:G:38:ASP:HB3	7:G:41:GLU:HB3	1.92	0.52	
2:B:346:ASP:N	2:B:347:PRO:HD3	2.25	0.51	
3:C:156:LEU:HD22	3:C:195:MET:HG3	1.92	0.51	
2:B:304:SER:HB3	2:B:350:ARG:CZ	2.40	0.51	
1:A:343:VAL:CG2	1:A:363:ILE:HD12	2.41	0.51	
2:B:326:LEU:HD23	2:B:326:LEU:O	2.11	0.51	
7:G:68:SER:O	7:G:71:VAL:HG12	2.10	0.51	
10:A:1022:HOH:O	4:D:34:THR:HG21	2.10	0.51	
3:C:173:ILE:HG22	3:C:175:GLU:HG2	1.92	0.51	
6:F:4:THR:HG23	6:F:55:ARG:NE	2.12	0.51	
2:B:189:ILE:HD11	2:B:265:LEU:HG	1.93	0.51	
2:B:160:GLY:HA3	9:B:1002:ATP:O2G	2.11	0.51	
2:B:319:ARG:NH1	7:G:17:ASP:OD2	2.44	0.51	
4:D:118:ARG:HD3	4:D:118:ARG:C	2.30	0.51	
4:D:129:PHE:CG	4:D:232:THR:HB	2.45	0.51	
4:D:202:HIS:O	4:D:203:ARG:HG3	2.10	0.51	
4:D:281:ARG:NH1	6:F:102:PHE:CZ	2.79	0.51	
5:E:149:PHE:CE2	5:E:156:PRO:HG3	2.46	0.51	
1:A:349:LEU:O	1:A:353:LEU:HD23	2.10	0.51	
2:B:155:VAL:HG21	2:B:286:ILE:CD1	2.41	0.50	
4:D:75:LEU:HD13	4:D:123:SER:N	2.26	0.50	
4:D:202:HIS:C	4:D:203:ARG:HG3	2.32	0.50	
3:C:48:LEU:HG	3:C:79:TRP:CE3	2.47	0.50	
4:D:53:THR:C	4:D:54:LYS:HD2	2.31	0.50	
5:E:124:GLN:O	5:E:128:VAL:HG23	2.12	0.50	
1:A:157:GLN:HB2	1:A:368:ILE:HD12	1.93	0.50	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.41	0.50
1:A:191:LYS:HB2	1:A:303:VAL:CG2	2.42	0.50
1:A:370:HIS:HD2	1:A:372:MET:N	2.10	0.50
2:B:302:VAL:CG2	2:B:350:ARG:HH22	2.18	0.50
4:D:150:GLU:HG2	4:D:167:THR:HA	1.92	0.50
3:C:193:GLU:CG	3:C:195:MET:CE	2.90	0.50
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.77	0.50
1:A:374:ARG:NH1	9:A:1001:ATP:C8	2.80	0.50
6:F:68:ASN:HD22	6:F:69:SER:N	2.08	0.50
7:G:20:ASP:OD1	7:G:22:ASN:HB2	2.11	0.50
1:A:192:HIS:CD2	1:A:192:HIS:N	2.80	0.50
1:A:389:GLU:CD	1:A:414:PHE:HB2	2.31	0.50
6:F:87:CYS:O	6:F:91:MET:HG2	2.11	0.50
4:D:19:PHE:HB3	4:D:106:LYS:HD3	1.94	0.50
3:C:184:PRO:HB2	3:C:231:ALA:HB1	1.93	0.49
4:D:263:HIS:HD2	4:D:266:MET:CE	2.24	0.49
2:B:231:GLN:O	2:B:235:LEU:HB2	2.11	0.49
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.42	0.49
3:C:107:ASN:C	3:C:107:ASN:ND2	2.66	0.49
3:C:212:ALA:HB3	3:C:255:GLU:OE2	2.13	0.49
3:C:125:PHE:HD2	3:C:132:TRP:CE2	2.30	0.49
3:C:119:VAL:HG21	3:C:136:HIS:HB3	1.95	0.49
4:D:199:LEU:HB2	4:D:224:THR:HB	1.95	0.49
1:A:191:LYS:HZ1	1:A:306:ASN:HD22	1.60	0.49
5:E:9:MET:HE3	5:E:13:THR:HB	1.93	0.49
3:C:254:THR:HG21	3:C:372:VAL:HG22	1.95	0.48
1:A:191:LYS:NZ	1:A:306:ASN:HD22	2.12	0.48
2:B:227:ILE:HD11	2:B:263:GLU:OE2	2.12	0.48
3:C:82:LYS:HG3	3:C:87:LYS:HG3	1.95	0.48
5:E:62:ASN:C	5:E:62:ASN:ND2	2.65	0.48
6:F:76:VAL:HG12	6:F:77:LYS:N	2.28	0.48
3:C:284:ARG:HD3	3:C:286:ASP:O	2.13	0.48
6:F:24:ASN:HD21	6:F:34:ASN:HD21	1.60	0.48
1:A:38:LYS:O	1:A:39:GLU:HB3	2.13	0.48
1:A:147:LEU:HD12	1:A:377:VAL:HG13	1.94	0.48
3:C:110:LYS:NZ	3:C:177:GLU:OE1	2.45	0.48
3:C:216:ARG:HH12	3:C:256:SER:HB3	1.79	0.48
5:E:111:PHE:HA	5:E:112:PRO:HD3	1.70	0.48
1:A:149:LEU:HD23	1:A:320:VAL:HG21	1.96	0.48
2:B:287:GLN:NE2	2:B:298:TYR:OH	2.46	0.48
1:A:260:ASN:O	1:A:264:LYS:N	2.46	0.48



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
5:E:58:TYR:CD1	5:E:168:PHE:HZ	2.32	0.48	
3:C:102:VAL:HA	3:C:112:ALA:O	2.14	0.47	
1:A:191:LYS:HE2	1:A:303:VAL:CG2	2.31	0.47	
1:A:243:ASN:ND2	5:E:47:TYR:CE1	2.81	0.47	
2:B:321:LEU:HD12	2:B:342:ILE:HD11	1.95	0.47	
5:E:95:MET:HG2	5:E:141:GLY:O	2.15	0.47	
6:F:86:LEU:HD22	6:F:149:MET:CE	2.45	0.47	
2:B:151:LEU:CD1	2:B:300:HIS:HD2	2.26	0.47	
2:B:184:ILE:HD12	2:B:185:ALA:H	1.76	0.47	
6:F:31:GLU:OE2	6:F:32:ARG:NE	2.41	0.47	
6:F:68:ASN:C	6:F:68:ASN:ND2	2.67	0.47	
1:A:135:ASN:OD1	1:A:135:ASN:O	2.33	0.47	
3:C:321:LEU:HD11	6:F:129:HIS:CE1	2.50	0.47	
1:A:114:GLU:O	1:A:144:GLN:HG3	2.14	0.47	
3:C:119:VAL:CG2	3:C:120:ILE:N	2.78	0.47	
3:C:332:ILE:HA	3:C:346:CYS:O	2.15	0.47	
4:D:129:PHE:CD2	4:D:237:ARG:HG3	2.49	0.47	
6:F:73:SER:HB3	6:F:112:TYR:CG	2.50	0.47	
7:G:91:ILE:O	7:G:95:VAL:HG23	2.15	0.47	
1:A:311:VAL:O	1:A:315:LEU:HG	2.15	0.46	
2:B:155:VAL:HG21	2:B:286:ILE:CG1	2.45	0.46	
4:D:68:GLN:HA	4:D:72:ALA:HB3	1.98	0.46	
1:A:289:ASN:C	1:A:289:ASN:ND2	2.69	0.46	
3:C:228:LEU:C	3:C:228:LEU:HD23	2.36	0.46	
3:C:254:THR:HG21	3:C:372:VAL:CG2	2.46	0.46	
2:B:155:VAL:HG21	2:B:286:ILE:HG12	1.97	0.46	
2:B:278:VAL:HG13	2:B:279:ALA:N	2.29	0.46	
2:B:326:LEU:HD23	2:B:326:LEU:C	2.36	0.46	
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.72	0.46	
1:A:384:LEU:HB3	1:A:414:PHE:CZ	2.50	0.46	
3:C:234:LYS:O	3:C:235:MET:HB2	2.16	0.46	
5:E:143:ARG:O	5:E:146:GLU:HG2	2.15	0.45	
1:A:21:TYR:OH	1:A:103:ALA:HB2	2.17	0.45	
4:D:67:LEU:HD13	4:D:120:CYS:O	2.16	0.45	
1:A:389:GLU:OE2	1:A:414:PHE:HB2	2.17	0.45	
2:B:171:GLU:OE2	2:B:171:GLU:HA	2.17	0.45	
3:C:109:LYS:HD3	3:C:176:VAL:O	2.16	0.45	
5:E:130:ARG:HG3	5:E:130:ARG:NH1	2.31	0.45	
5:E:23:PRO:HG3	5:E:33:PRO:HB2	1.99	0.45	
1:A:193:ILE:O	1:A:195:ILE:N	2.45	0.45	
1:A:239:VAL:HG23	1:A:240:LYS:N	2.31	0.45	



	A A A	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:398:LYS:HD2	10:A:1020:HOH:O	2.17	0.45	
3:C:73:ASP:O	3:C:74:ARG:HB2	2.16	0.45	
4:D:126:GLU:O	4:D:130:GLN:HB2	2.16	0.45	
7:G:78:ILE:O	7:G:82:VAL:HG23	2.16	0.45	
4:D:27:LYS:HD3	4:D:27:LYS:HA	1.88	0.45	
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.47	0.45	
6:F:44:LYS:HG2	10:F:193:HOH:O	2.17	0.45	
6:F:76:VAL:HG13	10:F:188:HOH:O	2.17	0.45	
5:E:82:LEU:HD13	5:E:95:MET:SD	2.57	0.44	
5:E:166:ARG:HG2	5:E:166:ARG:HH11	1.82	0.44	
3:C:107:ASN:HD22	3:C:109:LYS:H	1.65	0.44	
2:B:347:PRO:HA	2:B:348:PRO:HD3	1.75	0.44	
3:C:184:PRO:HB2	3:C:231:ALA:HB3	2.00	0.44	
6:F:125:GLN:HG2	6:F:125:GLN:H	1.59	0.44	
3:C:40:ASN:ND2	10:C:405:HOH:O	2.50	0.44	
5:E:113:LEU:HD21	5:E:171:LYS:HG3	2.00	0.44	
4:D:45:ILE:HA	4:D:56:MET:O	2.17	0.44	
2:B:310:TYR:CZ	9:B:1002:ATP:H2	2.36	0.44	
3:C:68:VAL:HG12	3:C:104:TRP:NE1	2.32	0.44	
2:B:146:LEU:CD1	2:B:169:VAL:HB	2.48	0.44	
3:C:263:HIS:CD2	6:F:21:CYS:HB3	2.53	0.43	
5:E:41:ILE:HG13	5:E:41:ILE:O	2.18	0.43	
3:C:174:LYS:HG3	3:C:175:GLU:N	2.33	0.43	
4:D:203:ARG:HH12	4:D:218:ASP:HA	1.79	0.43	
5:E:86:ASN:O	5:E:87:SER:HB3	2.18	0.43	
3:C:96:ASN:OD1	3:C:97:ARG:HG2	2.18	0.43	
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.99	0.43	
2:B:239:VAL:HG23	2:B:240:LEU:CD1	2.46	0.43	
4:D:170:LYS:HE2	4:D:170:LYS:CA	2.31	0.43	
4:D:208:GLU:HB3	10:D:327:HOH:O	2.18	0.43	
6:F:41:ARG:HB3	6:F:47:LEU:HD11	2.01	0.43	
3:C:258:LEU:O	3:C:269:LEU:HD12	2.19	0.43	
6:F:86:LEU:HD22	6:F:149:MET:HE3	1.99	0.43	
1:A:229:GLU:HG2	9:A:1001:ATP:C4	2.53	0.43	
4:D:14:THR:HG21	4:D:45:ILE:HG21	2.01	0.43	
4:D:137:GLU:OE1	4:D:158:LYS:HB2	2.19	0.43	
4:D:164:VAL:HG22	4:D:224:THR:HG23	2.00	0.43	
3:C:185:TRP:CD2	3:C:231:ALA:HB2	2.54	0.43	
5:E:84:LYS:HA	5:E:84:LYS:HD3	1.91	0.43	
7:G:83:LEU:HD22	7:G:128:TRP:CD2	2.53	0.43	
2:B:163:VAL:CG2	2:B:164:THR:N	2.81	0.43	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	$ ext{overlap}(ext{\AA})$
3:C:13:CYS:SG	3:C:58:VAL:HG23	2.58	0.43
3:C:321:LEU:N	3:C:321:LEU:CD1	2.81	0.43
6:F:85:ILE:HG13	6:F:86:LEU:N	2.33	0.43
7:G:55:LEU:HD22	7:G:94:ALA:HB1	2.01	0.42
5:E:14:LYS:O	5:E:15:LEU:HD23	2.19	0.42
6:F:8:TYR:OH	6:F:61:VAL:HG23	2.19	0.42
1:A:289:ASN:ND2	1:A:291:ASP:H	2.16	0.42
3:C:264:ASP:O	3:C:265:CYS:HB2	2.19	0.42
5:E:9:MET:SD	5:E:63:GLU:HG2	2.59	0.42
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.55	0.42
4:D:223:ILE:HG21	4:D:247:PHE:CE2	2.54	0.42
7:G:18:GLU:OE1	7:G:23:LYS:NZ	2.52	0.42
7:G:38:ASP:O	7:G:42:VAL:HG23	2.18	0.42
3:C:230:ASP:OD2	3:C:233:LYS:HG3	2.19	0.42
1:A:117:LEU:HD11	1:A:192:HIS:HE1	1.85	0.42
4:D:75:LEU:HD23	4:D:75:LEU:C	2.40	0.42
4:D:106:LYS:O	4:D:108:SER:N	2.52	0.42
5:E:18:ASN:O	5:E:63:GLU:HB3	2.20	0.42
5:E:105:ILE:HB	5:E:106:PRO:HD2	2.02	0.42
1:A:239:VAL:HG13	5:E:4:TYR:CZ	2.55	0.42
2:B:177:HIS:ND1	2:B:178:LEU:HG	2.35	0.42
2:B:246:LEU:HB3	2:B:247:PRO:HD2	2.01	0.42
3:C:266:PHE:CE1	3:C:284:ARG:HG3	2.55	0.42
4:D:54:LYS:HD2	4:D:54:LYS:N	2.33	0.42
1:A:2:ALA:HB2	1:A:391:TYR:CE1	2.55	0.42
1:A:19:LEU:HD23	1:A:19:LEU:N	2.34	0.42
3:C:179:ARG:HA	3:C:180:PRO:HD3	1.80	0.42
4:D:202:HIS:O	4:D:202:HIS:CG	2.73	0.42
4:D:205:PRO:HG3	4:D:222:TYR:CZ	2.55	0.42
4:D:223:ILE:HG21	4:D:247:PHE:CZ	2.54	0.42
7:G:99:ASP:O	7:G:102:GLY:N	2.52	0.42
1:A:234:VAL:HG11	1:A:334:ARG:HG2	2.01	0.42
1:A:237:ASP:OD2	1:A:240:LYS:HG3	2.20	0.41
1:A:61:PHE:C	1:A:66:ALA:HB2	2.41	0.41
1:A:319:ILE:HB	1:A:367:VAL:HG22	2.02	0.41
2:B:295:SER:O	2:B:299:LYS:HG2	2.21	0.41
3:C:366:LEU:HD12	3:C:366:LEU:N	2.35	0.41
5:E:66:ARG:HH11	5:E:66:ARG:HG3	1.85	0.41
1:A:152:SER:HB3	1:A:320:VAL:CG1	2.51	0.41
2:B:161:ASP:OD1	2:B:187:ARG:HG3	2.20	0.41
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.55	0.41



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
5:E:9:MET:HB2	5:E:62:ASN:OD1	2.20	0.41	
7:G:55:LEU:CD2	7:G:94:ALA:HB1	2.51	0.41	
7:G:100:LYS:HA	7:G:100:LYS:HD3	1.76	0.41	
1:A:242:PHE:CE1	5:E:50:LYS:HB3	2.56	0.41	
2:B:155:VAL:O	2:B:301:ILE:HA	2.20	0.41	
1:A:177:VAL:HG11	1:A:300:VAL:HA	2.01	0.41	
1:A:329:ARG:O	1:A:330:ASP:HB2	2.20	0.41	
2:B:153:THR:HA	2:B:169:VAL:O	2.21	0.41	
2:B:306:GLY:HA2	2:B:309:MET:CE	2.51	0.41	
4:D:134:GLU:HB2	4:D:136:LYS:HG3	2.03	0.41	
3:C:102:VAL:O	3:C:103:ARG:NH1	2.54	0.41	
3:C:286:ASP:HB2	3:C:357:TRP:CH2	2.56	0.41	
2:B:159:SER:HB2	2:B:164:THR:HG23	2.03	0.41	
3:C:34:ILE:HB	3:C:46:HIS:HB2	2.02	0.41	
3:C:92:ILE:HD12	3:C:92:ILE:N	2.36	0.41	
3:C:139:LYS:HA	3:C:140:PRO:HA	1.85	0.41	
3:C:183:THR:HG21	3:C:185:TRP:HD1	1.85	0.41	
4:D:263:HIS:O	4:D:267:ARG:HG3	2.20	0.41	
5:E:144:LEU:HD13	5:E:144:LEU:O	2.21	0.41	
6:F:161:ALA:O	6:F:165:LEU:HB2	2.20	0.41	
7:G:114:PHE:CZ	7:G:126:LEU:HD23	2.56	0.41	
3:C:17:ASN:HB3	3:C:60:TRP:CZ2	2.56	0.41	
3:C:69:THR:O	3:C:76:ALA:HA	2.21	0.41	
4:D:181:PHE:CE2	6:F:157:ALA:HA	2.55	0.41	
6:F:33:HIS:ND1	6:F:35:LYS:HE2	2.35	0.41	
7:G:66:THR:O	7:G:72:LYS:HE3	2.21	0.41	
4:D:267:ARG:HG2	6:F:93:PHE:HZ	1.86	0.40	
5:E:81:LYS:HE2	5:E:98:LEU:HD21	2.03	0.40	
1:A:340:LYS:HE3	1:A:340:LYS:HB3	1.95	0.40	
2:B:317:LEU:HB2	2:B:344:ILE:HD12	2.03	0.40	
3:C:172:TYR:C	3:C:172:TYR:CD2	2.92	0.40	
6:F:35:LYS:NZ	10:F:171:HOH:O	2.54	0.40	
1:A:129:ILE:O	1:A:133:SER:HB2	2.21	0.40	
1:A:157:GLN:HB3	1:A:366:GLN:NE2	2.36	0.40	
1:A:247:THR:O	1:A:247:THR:HG22	2.20	0.40	
2:B:319:ARG:O	2:B:323:GLN:HG3	2.22	0.40	
3:C:29:ASN:O	3:C:54:GLN:HA	2.21	0.40	
3:C:273:ASP:O	3:C:277:GLY:N	2.51	0.40	
6:F:30:VAL:HG11	6:F:33:HIS:CE1	2.56	0.40	
6:F:138:PHE:O	6:F:142:ILE:HG23	2.22	0.40	
1:A:128:GLU:HG3	1:A:132:GLU:HG3	2.03	0.40	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:C:207:GLY:O	3:C:219:TRP:HA	2.22	0.40
4:D:248:ARG:HD3	4:D:248:ARG:C	2.42	0.40
1:A:311:VAL:O	1:A:311:VAL:HG22	2.21	0.40
5:E:18:ASN:ND2	5:E:118:ALA:HB2	2.37	0.40
5:E:45:ALA:HA	5:E:68:LEU:HD11	2.03	0.40
5:E:158:LYS:HA	5:E:161:THR:OG1	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	Perce	entiles
1	А	393/418~(94%)	371 (94%)	20~(5%)	2(0%)	29	40
2	В	206/394~(52%)	184 (89%)	18 (9%)	4 (2%)	8	9
3	С	338/372~(91%)	312 (92%)	24 (7%)	2(1%)	25	34
4	D	270/300~(90%)	260 (96%)	9(3%)	1 (0%)	34	46
5	E	165/178~(93%)	152 (92%)	12 (7%)	1 (1%)	25	34
6	F	164/168~(98%)	160 (98%)	3 (2%)	1 (1%)	25	34
7	G	130/151~(86%)	123~(95%)	6 (5%)	1 (1%)	19	27
All	All	1666/1981~(84%)	1562 (94%)	92 (6%)	12 (1%)	22	30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	249	GLY
2	В	329	VAL
2	В	331	LYS
6	F	102	PHE
5	Е	87	SER



Continued from previous page...

Mol	Chain	Res	Type
2	В	179	THR
3	С	50	GLU
4	D	107	ASP
1	А	194	PRO
2	В	342	ILE
3	С	62	PRO
7	G	16	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	entiles
1	А	339/363~(93%)	326~(96%)	13 (4%)	33	45
2	В	154/345~(45%)	147 (96%)	7 (4%)	27	37
3	С	288/313~(92%)	279~(97%)	9~(3%)	40	54
4	D	241/264~(91%)	235~(98%)	6 (2%)	47	62
5	Ε	152/159~(96%)	141 (93%)	11 (7%)	14	18
6	F	153/155~(99%)	144 (94%)	9~(6%)	19	25
7	G	109/124~(88%)	105 (96%)	4 (4%)	34	46
All	All	1436/1723~(83%)	1377 (96%)	59(4%)	30	41

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	19	LEU
1	А	68	GLU
1	А	88	LEU
1	А	143	VAL
1	А	191	LYS
1	А	230	ARG
1	А	255	GLN
1	А	268	SER
1	А	289	ASN
1	А	310	ASP



Mol	Chain	Res	Type
1	А	318	ASN
1	А	335	LEU
1	А	394	CYS
2	В	182	LEU
2	В	183	ASP
2	В	184	ILE
2	В	200	ARG
2	В	220	LEU
2	В	274	GLU
2	В	281	LEU
3	С	21	THR
3	С	30	HIS
3	С	90	LEU
3	С	107	ASN
3	С	140	PRO
3	С	183	THR
3	С	284	ARG
3	С	321	LEU
3	С	370	LYS
4	D	116	LEU
4	D	141	ARG
4	D	157	LYS
4	D	172	ASP
4	D	245	HIS
4	D	281	ARG
5	Ε	10	ASP
5	Е	22	LEU
5	Е	25	ARG
5	E	62	ASN
5	Е	82	LEU
5	Е	95	MET
5	Е	98	LEU
5	Е	102	ASN
5	Е	130	ARG
5	Е	133	LEU
5	Е	161	THR
6	F	6	ARG
6	F	68	ASN
6	F	85	ILE
6	F	101	PHE
6	F	125	GLN
6	F	128	LYS



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Mol	Chain	Res	Type
6	F	143	ASP
6	F	165	LEU
6	F	166	LYS
7	G	39	GLU
7	G	69	GLN
7	G	87	LYS
7	G	90	ASP

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such side chains are listed below:

Mol	Chain	Res	Type
1	А	122	ASN
1	А	157	GLN
1	А	176	HIS
1	А	205	GLN
1	А	206	GLN
1	А	255	GLN
1	А	289	ASN
1	А	306	ASN
1	А	318	ASN
1	А	366	GLN
1	А	370	HIS
1	А	395	HIS
2	В	205	ASN
2	В	229	GLN
2	В	231	GLN
2	В	284	ASN
2	В	287	GLN
2	В	323	GLN
3	С	22	GLN
3	С	29	ASN
3	С	33	HIS
3	С	44	GLN
3	С	46	HIS
3	С	54	GLN
3	С	65	ASN
3	С	107	ASN
3	С	331	GLN
4	D	21	ASN
4	D	26	ASN
4	D	49	ASN
4	D	140	ASN



Mol	Chain	\mathbf{Res}	Type
4	D	202	HIS
4	D	231	HIS
4	D	263	HIS
5	Е	62	ASN
5	Е	83	GLN
6	F	24	ASN
6	F	28	GLN
6	F	68	ASN
6	F	125	GLN
6	F	137	HIS
7	G	50	ASN
7	G	56	GLN
7	G	96	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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).

Mal	Tuno	Chain	Dog	Link	Bo	ond leng	ths	B	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ATP	В	1002	8	26,33,33	1.35	3 (11%)	31,52,52	1.57	4 (12%)



Mal	Type	Chain	Dog	Link	Bo	ond leng	\mathbf{ths}	B	ond ang	les
	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
9	ATP	А	1001	8	$26,\!33,\!33$	1.34	3 (11%)	31,52,52	1.64	5 (16%)

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
9	ATP	В	1002	8	-	2/18/38/38	0/3/3/3
9	ATP	А	1001	8	-	2/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
9	А	1001	ATP	C2-N1	3.58	1.40	1.33
9	В	1002	ATP	C2-N1	3.54	1.40	1.33
9	В	1002	ATP	PG-01G	3.37	1.61	1.50
9	А	1001	ATP	PG-01G	3.37	1.61	1.50
9	В	1002	ATP	O4'-C1'	2.29	1.44	1.41
9	А	1001	ATP	O4'-C1'	2.05	1.43	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
9	А	1001	ATP	N3-C2-N1	-5.46	120.15	128.68
9	В	1002	ATP	N3-C2-N1	-5.29	120.41	128.68
9	А	1001	ATP	PA-O3A-PB	-3.30	121.50	132.83
9	В	1002	ATP	PB-O3B-PG	-3.21	121.81	132.83
9	А	1001	ATP	O4'-C1'-C2'	-3.21	102.23	106.93
9	В	1002	ATP	PA-O3A-PB	-3.08	122.26	132.83
9	А	1001	ATP	PB-O3B-PG	-3.04	122.41	132.83
9	В	1002	ATP	O3G-PG-O3B	2.60	113.35	104.64
9	А	1001	ATP	O3G-PG-O3B	2.56	113.20	104.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	А	1001	ATP	PB-O3B-PG-O2G
9	В	1002	ATP	PB-O3B-PG-O2G



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Mol	Chain	Res	Type	Atoms
9	А	1001	ATP	PB-O3B-PG-O1G
9	В	1002	ATP	PB-O3B-PG-O1G

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	В	1002	ATP	4	0
9	А	1001	ATP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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 (i)

6.1 Protein, DNA and RNA chains (i)

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	А	399/418~(95%)	0.31	21 (5%) 26 31	23, 49, 76, 102	0
2	В	208/394~(52%)	0.56	29~(13%) 2 3	31, 60, 92, 100	0
3	С	342/372~(91%)	0.02	13 (3%) 40 47	27, 40, 67, 89	0
4	D	274/300~(91%)	0.16	9 (3%) 46 53	26, 44, 69, 82	0
5	Е	169/178~(94%)	0.56	17 (10%) 7 8	40, 57, 81, 92	0
6	F	166/168~(98%)	-0.09	4 (2%) 59 65	28, 41, 55, 73	0
7	G	134/151~(88%)	0.75	18 (13%) 3 4	32, 66, 85, 105	0
All	All	1692/1981~(85%)	0.28	111 (6%) 18 21	23, 47, 83, 105	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	35	ALA	5.6
1	А	418	SER	5.2
1	А	72	TYR	5.1
1	А	351	GLU	5.0
7	G	66	THR	4.9
2	В	350	ARG	4.8
1	А	353	LEU	4.8
3	С	1	MET	4.4
1	А	348	LYS	4.2
5	Ε	109	PRO	4.1
5	Е	71	ILE	3.8
1	А	417	MET	3.8
1	А	159	GLY	3.8
2	В	334	VAL	3.8
1	А	156	ARG	3.7
2	В	288	ALA	3.7
7	G	25	VAL	3.6



Mol	Chain	Res	Type	RSRZ
2	В	292	ASP	3.6
7	G	44	SER	3.6
7	G	65	ASN	3.6
7	G	49	GLY	3.5
1	А	349	LEU	3.5
4	D	202	HIS	3.5
1	А	347	LEU	3.4
1	А	352	GLU	3.4
5	Е	49	PHE	3.3
5	Е	85	CYS	3.3
2	В	293	THR	3.3
2	В	150	GLY	3.3
6	F	3	ALA	3.2
3	С	367	LYS	3.2
1	А	70	PRO	3.2
5	Е	93	LYS	3.2
5	Е	38	ASP	3.2
7	G	63	PRO	3.2
7	G	13	LYS	3.1
7	G	19	TYR	3.1
5	Е	86	ASN	3.1
5	Е	37	LYS	3.1
1	А	39	GLU	3.1
5	Е	90	GLN	3.0
5	Е	75	ILE	3.0
5	Е	96	TYR	3.0
7	G	71	VAL	2.9
1	А	157	GLN	2.8
2	В	333	ASP	2.7
1	А	2	ALA	2.7
2	В	174	SER	2.7
3	С	130	ASP	2.7
2	В	178	LEU	2.7
2	В	274	GLU	2.7
4	D	218	ASP	2.7
5	Е	150	ASP	2.7
7	G	45	CYS	2.6
3	С	127	GLN	2.6
2	В	173	PHE	2.6
2	В	273	VAL	2.6
7	G	89	ASN	2.6
7	G	43	ASP	2.6



Mol	Chain	Res	Type	RSRZ
3	C	319	ALA	2.5
2	В	151	LEU	2.5
7	G	21	GLU	2.5
1	А	71	THR	2.5
7	G	11	PHE	2.5
7	G	47	ARG	2.5
1	А	291	ASP	2.5
1	А	168	ILE	2.5
1	А	158	VAL	2.5
2	В	282	LEU	2.5
4	D	275	LYS	2.5
2	В	171	GLU	2.4
5	Е	70	TYR	2.4
3	С	129	ASN	2.4
2	В	347	PRO	2.4
4	D	203	ARG	2.4
3	С	370	LYS	2.4
3	С	287	VAL	2.4
2	В	169	VAL	2.3
3	С	208	VAL	2.3
3	С	321	LEU	2.3
4	D	217	GLY	2.3
2	В	272	ASN	2.3
5	Е	100	ILE	2.3
6	F	63	ILE	2.3
7	G	14	VAL	2.2
2	В	183	ASP	2.2
2	В	148	ALA	2.2
4	D	121	PHE	2.2
1	А	202	TYR	2.2
2	В	147	TYR	2.2
2	В	170	TYR	2.2
4	D	204	GLU	2.2
5	Е	89	SER	2.2
3	С	209	CYS	2.2
2	В	143	VAL	2.1
2	В	152	LEU	2.1
2	В	265	LEU	2.1
2	В	317	LEU	2.1
6	F	19	ALA	2.1
5	Е	73	LEU	2.1
4	D	260	ALA	2.1



Mol	Chain	Res	Type	RSRZ
1	А	388	PRO	2.1
3	С	84	ARG	2.1
2	В	154	GLY	2.1
4	D	246	THR	2.1
3	С	125	PHE	2.1
7	G	46	LEU	2.1
6	F	6	ARG	2.1
2	В	278	VAL	2.0
2	В	176	PRO	2.0
5	Е	10	ASP	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 monosaccharides 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, 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
8	CA	В	501	1/1	0.88	0.10	$95,\!95,\!95,\!95$	0
9	ATP	В	1002	31/31	0.95	0.16	52,59,74,76	0
8	CA	А	500	1/1	0.96	0.30	73,73,73,73	0
9	ATP	А	1001	31/31	0.97	0.14	46,52,58,60	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

