



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:20 pm BST

PDB ID : 1H1V
Title : gelsolin G4-G6/actin complex
Authors : Choe, H.; Burtnick, L.D.; Mejillano, M.; Yin, H.L.; Robinson, R.C.; Choe, S.
Deposited on : 2002-07-23
Resolution : 2.99 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

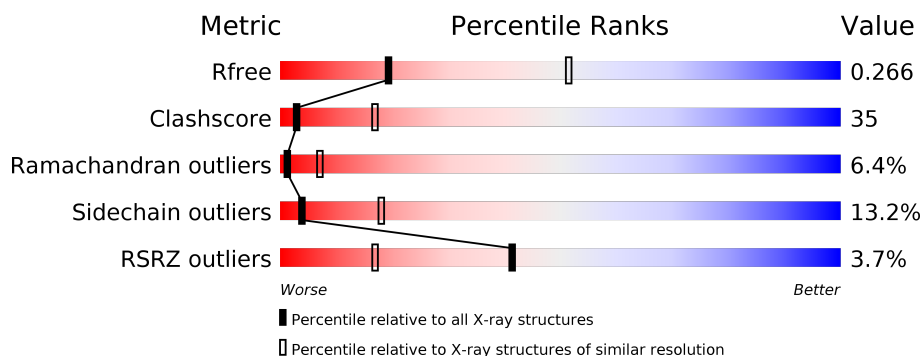
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	375	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>35%</div> <div>8%</div> <div>..</div> </div> </div>
2	G	331	<div> <div>5%</div> <div> <div></div> <div>44%</div> <div>38%</div> <div>14%</div> <div>..</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5796 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2875	1822	485	547	21			

- Molecule 2 is a protein called GELSOLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	327	Total	C	N	O	S	0	0	0
			2539	1600	437	495	7			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	4	Total	Ca	0	0
			4	4		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.35Å 113.45Å 159.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 – 2.99 19.72 – 2.99	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.73-2.99) 98.0 (19.72-2.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.98Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , 0.268 0.218 , 0.266	Depositor DCC
R_{free} test set	1010 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5796	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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: CA, ATP

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	0.68	0/2937	0.86	14/3977 (0.4%)
2	G	0.61	0/2598	0.88	10/3525 (0.3%)
All	All	0.65	0/5535	0.87	24/7502 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ASP	CB-CG-OD2	7.37	124.93	118.30
1	A	288	ASP	CB-CG-OD2	6.65	124.28	118.30
2	G	737	ASP	CB-CG-OD2	6.62	124.26	118.30
2	G	665	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	286	ASP	CB-CG-OD2	6.55	124.20	118.30
1	A	80	ASP	CB-CG-OD2	6.35	124.02	118.30
2	G	620	GLY	N-CA-C	6.23	128.68	113.10
1	A	184	ASP	CB-CG-OD2	6.19	123.88	118.30
2	G	414	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	179	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	51	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	363	ASP	CB-CG-OD2	5.59	123.33	118.30
2	G	612	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	24	ASP	CB-CG-OD2	5.35	123.12	118.30
2	G	738	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	211	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	244	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	25	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	81	ASP	CB-CG-OD2	5.15	122.94	118.30
2	G	573	SER	N-CA-C	-5.08	97.27	111.00
2	G	712	ASP	CB-CG-OD2	5.07	122.86	118.30
2	G	415	ASP	CB-CG-OD2	5.03	122.83	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	LEU	CA-CB-CG	-5.02	103.75	115.30
2	G	636	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2875	0	2846	147	2
2	G	2539	0	2454	226	1
3	A	1	0	0	0	0
3	G	4	0	0	0	0
4	A	31	0	12	1	0
5	A	196	0	0	12	1
5	G	150	0	0	15	2
All	All	5796	0	5312	373	3

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 35.

All (373) 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:47:MET:SD	5:A:2018:HOH:O	2.00	1.17
1:A:47:MET:HA	5:A:2018:HOH:O	1.49	1.13
1:A:47:MET:CA	5:A:2018:HOH:O	1.99	1.10
1:A:53:TYR:HE2	1:A:57:GLU:CB	1.63	1.10
1:A:39:ARG:HG2	1:A:65:LEU:H	1.19	1.07
2:G:413:ASP:OD1	5:G:2032:HOH:O	1.71	1.05
1:A:53:TYR:CE2	1:A:57:GLU:CB	2.40	1.04
2:G:564:ASN:HD21	2:G:635:MET:HE2	1.21	1.02
2:G:625:ARG:NH1	5:G:2093:HOH:O	1.93	1.01
1:A:330:ILE:HG22	1:A:332:PRO:HD3	1.45	0.98
2:G:595:LEU:HD13	2:G:602:PRO:HG3	1.45	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:708:PRO:O	2:G:710:ASN:N	1.97	0.97
1:A:47:MET:CG	5:A:2018:HOH:O	2.13	0.96
1:A:123:MET:O	1:A:129:VAL:HG22	1.64	0.95
2:G:598:LEU:O	2:G:599:ARG:HB2	1.66	0.95
2:G:708:PRO:C	2:G:710:ASN:H	1.64	0.94
2:G:707:ASP:HB2	2:G:711:ARG:CB	1.98	0.91
1:A:45:VAL:HG12	1:A:46:GLY:H	1.32	0.91
2:G:598:LEU:O	2:G:599:ARG:CB	2.19	0.91
2:G:545:SER:O	5:G:2077:HOH:O	1.86	0.90
2:G:595:LEU:HD13	2:G:602:PRO:CG	2.01	0.90
1:A:227:MET:HE1	1:A:256:ARG:HD2	1.50	0.90
2:G:707:ASP:OD2	2:G:709:ALA:HA	1.71	0.90
2:G:564:ASN:ND2	2:G:635:MET:CE	2.36	0.89
1:A:51:ASP:OD1	1:A:52:SER:OG	1.88	0.89
2:G:525:SER:O	2:G:527:GLU:N	2.04	0.89
2:G:564:ASN:HD21	2:G:635:MET:CE	1.86	0.88
2:G:707:ASP:HB2	2:G:711:ARG:HB3	1.52	0.88
2:G:595:LEU:CD1	2:G:602:PRO:HG3	2.02	0.88
2:G:526:ARG:HH11	2:G:526:ARG:HG2	1.38	0.87
1:A:39:ARG:CG	1:A:65:LEU:H	1.86	0.86
2:G:493:THR:N	2:G:494:PRO:HD2	1.90	0.86
2:G:526:ARG:CG	2:G:526:ARG:HH11	1.89	0.85
1:A:61:LYS:O	1:A:62:ARG:HB2	1.77	0.85
1:A:36:GLY:O	1:A:37:ARG:HG3	1.76	0.85
2:G:564:ASN:ND2	2:G:635:MET:HE2	1.90	0.84
2:G:710:ASN:OD1	5:G:2134:HOH:O	1.96	0.84
1:A:45:VAL:CG1	1:A:46:GLY:H	1.91	0.83
1:A:65:LEU:HD23	1:A:65:LEU:N	1.94	0.82
2:G:437:THR:HA	2:G:440:GLN:HE21	1.45	0.81
2:G:424:ARG:NH2	2:G:524:THR:HG23	1.95	0.81
2:G:562:ASN:OD1	2:G:564:ASN:N	2.11	0.81
2:G:713:ARG:O	2:G:714:ARG:NH1	2.15	0.80
1:A:65:LEU:HG	1:A:66:THR:N	1.99	0.78
1:A:65:LEU:O	1:A:66:THR:HG23	1.84	0.78
1:A:39:ARG:HG2	1:A:65:LEU:N	1.99	0.77
2:G:707:ASP:C	2:G:709:ALA:H	1.87	0.77
1:A:37:ARG:O	1:A:65:LEU:HA	1.85	0.77
1:A:27:PRO:HD3	1:A:340:TRP:CE3	2.20	0.77
1:A:220:ALA:HB1	1:A:226:GLU:HG3	1.65	0.76
2:G:708:PRO:C	2:G:710:ASN:N	2.36	0.76
2:G:493:THR:H	2:G:494:PRO:HD2	1.50	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:620:GLY:O	2:G:621:LYS:CB	2.35	0.75
1:A:34:ILE:HD11	1:A:59:GLN:HG2	1.68	0.75
2:G:707:ASP:O	2:G:709:ALA:N	2.19	0.74
2:G:564:ASN:ND2	2:G:635:MET:HE1	2.03	0.74
2:G:626:THR:O	5:G:2094:HOH:O	2.04	0.74
2:G:449:ILE:HG23	2:G:464:TYR:HB2	1.70	0.73
2:G:594:LEU:O	2:G:594:LEU:HD22	1.88	0.73
2:G:538:LEU:HD11	2:G:567:PHE:HB3	1.71	0.73
1:A:358:THR:OG1	1:A:361:GLU:HG3	1.89	0.72
1:A:45:VAL:HG12	1:A:46:GLY:N	2.03	0.72
2:G:525:SER:HB3	5:G:2068:HOH:O	1.88	0.72
1:A:123:MET:O	1:A:129:VAL:CG2	2.35	0.72
1:A:297:ASN:OD1	5:A:2156:HOH:O	2.08	0.71
2:G:704:ILE:O	2:G:705:GLU:HB2	1.90	0.71
1:A:61:LYS:O	1:A:62:ARG:CB	2.37	0.71
2:G:449:ILE:HD11	2:G:511:LEU:HD23	1.72	0.71
1:A:218:TYR:OH	1:A:226:GLU:OE2	2.08	0.71
1:A:62:ARG:HG2	1:A:65:LEU:HD13	1.71	0.71
1:A:116:ARG:O	1:A:120:THR:OG1	2.10	0.70
1:A:46:GLY:O	5:A:2018:HOH:O	2.08	0.70
2:G:730:VAL:CG1	2:G:736:TRP:CD2	2.75	0.70
2:G:554:VAL:CG1	5:G:2081:HOH:O	2.40	0.70
2:G:621:LYS:O	2:G:622:ALA:CB	2.40	0.70
2:G:493:THR:N	2:G:494:PRO:CD	2.55	0.70
2:G:455:HIS:O	5:G:2042:HOH:O	2.08	0.70
2:G:426:GLU:HG3	2:G:431:VAL:HG22	1.75	0.69
2:G:705:GLU:C	2:G:707:ASP:H	1.95	0.69
1:A:59:GLN:O	1:A:61:LYS:N	2.26	0.69
2:G:571:THR:O	2:G:573:SER:N	2.26	0.69
2:G:620:GLY:O	2:G:621:LYS:HB2	1.91	0.69
2:G:498:ARG:NH2	5:G:2060:HOH:O	2.26	0.68
1:A:62:ARG:CZ	1:A:203:THR:HG21	2.24	0.68
2:G:487:ASP:OD1	2:G:492:GLY:HA2	1.93	0.68
2:G:577:LEU:HD13	2:G:604:GLN:NE2	2.07	0.68
2:G:672:MET:HB2	2:G:683:TRP:HB3	1.76	0.68
2:G:558:ALA:HB1	2:G:622:ALA:HA	1.75	0.67
1:A:44:MET:HG3	1:A:45:VAL:N	2.09	0.67
2:G:562:ASN:C	2:G:562:ASN:OD1	2.33	0.67
2:G:426:GLU:CD	2:G:431:VAL:HG21	2.15	0.67
2:G:430:LYS:HG3	2:G:430:LYS:O	1.95	0.66
1:A:193:LEU:O	1:A:196:ARG:HB3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:707:ASP:OD2	2:G:709:ALA:CA	2.43	0.66
1:A:73:HIS:HA	1:A:159:VAL:HG13	1.76	0.66
2:G:656:GLU:O	2:G:658:PRO:HD3	1.96	0.66
1:A:78:ASN:ND2	1:A:81:ASP:OD2	2.28	0.66
2:G:419:GLN:NE2	5:G:2037:HOH:O	2.29	0.66
1:A:45:VAL:CG1	1:A:46:GLY:N	2.59	0.65
2:G:621:LYS:O	2:G:622:ALA:HB3	1.96	0.65
2:G:472:THR:O	2:G:476:VAL:HG23	1.96	0.65
1:A:372:ARG:NH2	5:A:2193:HOH:O	2.29	0.65
2:G:660:GLU:O	2:G:662:MET:HG3	1.97	0.65
2:G:664:GLU:HG2	2:G:740:TYR:OH	1.97	0.65
2:G:518:ILE:HD13	2:G:594:LEU:HD23	1.77	0.65
1:A:50:LYS:H	1:A:50:LYS:HE3	1.62	0.64
2:G:554:VAL:HG12	5:G:2081:HOH:O	1.94	0.64
2:G:526:ARG:O	2:G:527:GLU:OE2	2.15	0.64
2:G:424:ARG:NH1	2:G:426:GLU:OE2	2.30	0.63
1:A:170:ALA:O	1:A:172:PRO:HD3	1.98	0.63
2:G:645:CYS:SG	2:G:673:LEU:HD23	2.38	0.63
1:A:136:ILE:N	1:A:136:ILE:HD12	2.13	0.63
2:G:431:VAL:O	2:G:431:VAL:HG23	1.99	0.63
2:G:651:ARG:HH11	2:G:651:ARG:HB2	1.64	0.63
1:A:53:TYR:CD2	1:A:57:GLU:CB	2.82	0.62
2:G:527:GLU:OE2	2:G:527:GLU:HA	1.98	0.62
2:G:707:ASP:C	2:G:709:ALA:N	2.53	0.62
2:G:526:ARG:HG2	2:G:526:ARG:NH1	2.07	0.62
1:A:210:ARG:O	1:A:214:GLU:HG3	1.99	0.62
2:G:598:LEU:O	2:G:599:ARG:CG	2.49	0.61
1:A:34:ILE:CD1	1:A:59:GLN:HG2	2.30	0.61
2:G:540:GLN:HG3	2:G:567:PHE:CZ	2.36	0.61
2:G:632:ASP:OD1	2:G:634:LYS:HD2	2.01	0.61
1:A:87:HIS:NE2	1:A:91:TYR:CD1	2.70	0.60
2:G:420:LYS:NZ	2:G:511:LEU:O	2.20	0.60
1:A:194:THR:HA	1:A:198:TYR:O	2.02	0.60
2:G:534:ALA:O	2:G:535:SER:HB3	2.00	0.60
1:A:46:GLY:C	5:A:2018:HOH:O	2.39	0.59
2:G:599:ARG:O	2:G:600:ALA:HB2	2.00	0.59
2:G:499:VAL:HA	5:G:2064:HOH:O	2.01	0.59
2:G:426:GLU:CG	2:G:431:VAL:HG22	2.32	0.59
1:A:205:GLU:HA	1:A:208:ILE:HG13	1.84	0.59
2:G:622:ALA:O	2:G:623:ALA:CB	2.51	0.59
1:A:352:PHE:O	1:A:355:MET:N	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:540:GLN:HE22	2:G:542:ARG:HH12	1.49	0.58
2:G:540:GLN:HE22	2:G:542:ARG:NH1	2.01	0.58
2:G:598:LEU:C	2:G:599:ARG:HG2	2.24	0.58
1:A:330:ILE:HG22	1:A:332:PRO:CD	2.28	0.58
2:G:467:GLN:HG2	2:G:476:VAL:HG13	1.86	0.58
2:G:595:LEU:HD13	2:G:602:PRO:CD	2.34	0.58
1:A:65:LEU:CG	1:A:66:THR:N	2.58	0.58
2:G:515:LYS:N	2:G:515:LYS:HD2	2.19	0.58
2:G:426:GLU:HG3	2:G:431:VAL:CG2	2.34	0.57
2:G:713:ARG:NH1	5:G:2136:HOH:O	2.37	0.57
1:A:9:VAL:HG21	1:A:344:SER:HA	1.86	0.57
2:G:629:ARG:NH2	2:G:638:HIS:O	2.38	0.57
2:G:598:LEU:O	2:G:599:ARG:HG2	2.04	0.57
2:G:620:GLY:O	2:G:621:LYS:CG	2.53	0.57
2:G:622:ALA:O	2:G:623:ALA:HB3	2.05	0.57
1:A:220:ALA:CB	1:A:226:GLU:HG3	2.34	0.56
2:G:424:ARG:O	2:G:426:GLU:HG2	2.05	0.56
1:A:352:PHE:HE2	1:A:356:TRP:CZ3	2.24	0.56
2:G:635:MET:SD	2:G:732:TRP:CZ3	2.99	0.56
2:G:526:ARG:O	2:G:526:ARG:HD2	2.05	0.55
2:G:544:ASN:HD21	2:G:548:ALA:HB3	1.72	0.55
2:G:427:GLY:HA3	2:G:526:ARG:HG2	1.88	0.55
2:G:455:HIS:CG	2:G:455:HIS:O	2.60	0.55
2:G:574:ALA:O	2:G:575:ALA:HB2	2.06	0.55
1:A:305:MET:HA	1:A:335:ARG:NH1	2.22	0.55
1:A:250:ILE:HG12	1:A:250:ILE:O	2.06	0.54
1:A:304:THR:O	1:A:335:ARG:NH1	2.40	0.54
2:G:589:THR:HG22	2:G:590:GLY:N	2.22	0.54
2:G:635:MET:SD	2:G:732:TRP:CH2	3.00	0.54
2:G:538:LEU:HD12	2:G:539:PHE:H	1.71	0.54
1:A:62:ARG:HG2	1:A:65:LEU:CD1	2.35	0.54
1:A:65:LEU:N	1:A:65:LEU:CD2	2.64	0.54
2:G:437:THR:CA	2:G:440:GLN:HE21	2.18	0.54
2:G:527:GLU:OE2	2:G:527:GLU:CA	2.56	0.54
2:G:431:VAL:O	2:G:431:VAL:CG2	2.56	0.54
2:G:707:ASP:CB	2:G:711:ARG:HB3	2.32	0.54
2:G:424:ARG:CZ	2:G:524:THR:HG23	2.38	0.54
2:G:493:THR:H	2:G:494:PRO:CD	2.17	0.54
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.90	0.53
2:G:620:GLY:O	2:G:621:LYS:HG3	2.08	0.53
1:A:162:ASN:HB2	1:A:176:MET:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLN:C	1:A:61:LYS:N	2.61	0.53
2:G:645:CYS:O	2:G:670:ASP:HB3	2.09	0.53
2:G:737:ASP:O	2:G:738:ASP:C	2.47	0.53
2:G:433:VAL:O	2:G:438:TYR:HE2	1.91	0.53
2:G:667:ALA:H	2:G:672:MET:HE1	1.74	0.53
1:A:276:GLU:OE1	5:A:2142:HOH:O	2.18	0.53
2:G:737:ASP:OD2	2:G:739:ASP:O	2.27	0.53
2:G:455:HIS:HE1	2:G:460:GLY:N	2.07	0.53
1:A:39:ARG:CG	1:A:65:LEU:N	2.65	0.53
2:G:603:VAL:O	2:G:604:GLN:C	2.47	0.53
1:A:257:CYS:HB3	1:A:258:PRO:CD	2.39	0.53
2:G:571:THR:O	2:G:572:PRO:C	2.47	0.52
1:A:107:GLU:OE2	1:A:116:ARG:NH1	2.39	0.52
2:G:647:ASN:C	2:G:647:ASN:ND2	2.63	0.52
1:A:264:PRO:HG2	1:A:272:ALA:O	2.09	0.52
2:G:437:THR:O	2:G:438:TYR:C	2.45	0.52
1:A:155:SER:HB2	1:A:160:THR:HG23	1.91	0.52
1:A:352:PHE:O	1:A:353:GLN:C	2.48	0.52
2:G:577:LEU:HD13	2:G:604:GLN:HE22	1.73	0.52
2:G:584:SER:O	2:G:588:LYS:HG3	2.08	0.52
2:G:540:GLN:NE2	2:G:542:ARG:NH1	2.57	0.52
1:A:87:HIS:CD2	1:A:91:TYR:CD1	2.98	0.52
2:G:415:ASP:HB3	2:G:417:THR:HG23	1.91	0.52
2:G:427:GLY:HA3	2:G:526:ARG:NH1	2.24	0.51
1:A:44:MET:CG	1:A:45:VAL:N	2.73	0.51
2:G:435:PRO:HA	2:G:438:TYR:CE2	2.45	0.51
2:G:489:GLU:HG2	2:G:490:LEU:HD12	1.91	0.51
2:G:642:LEU:HB2	2:G:661:LEU:HD22	1.92	0.51
2:G:643:PHE:HB2	2:G:673:LEU:HB2	1.92	0.51
2:G:534:ALA:O	2:G:535:SER:CB	2.59	0.50
2:G:561:LEU:HD23	2:G:578:TRP:CE2	2.47	0.50
2:G:599:ARG:O	2:G:600:ALA:CB	2.58	0.50
2:G:730:VAL:HG13	2:G:736:TRP:CD2	2.47	0.50
1:A:314:GLN:HB2	1:A:329:ILE:HD13	1.92	0.50
1:A:297:ASN:HB2	1:A:328:LYS:O	2.11	0.50
1:A:65:LEU:HD23	1:A:65:LEU:H	1.74	0.50
2:G:535:SER:O	2:G:536:THR:HB	2.11	0.50
2:G:542:ARG:HG2	2:G:543:ALA:N	2.26	0.50
1:A:96:VAL:HB	1:A:101:HIS:NE2	2.26	0.50
1:A:330:ILE:HD12	1:A:330:ILE:N	2.27	0.49
1:A:59:GLN:C	1:A:61:LYS:H	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:426:GLU:CD	2:G:431:VAL:CG2	2.80	0.49
2:G:725:GLU:CD	2:G:725:GLU:H	2.16	0.49
2:G:737:ASP:O	2:G:739:ASP:N	2.45	0.49
1:A:203:THR:HA	1:A:206:ARG:NH1	2.28	0.49
2:G:544:ASN:ND2	2:G:548:ALA:HB3	2.26	0.49
1:A:109:PRO:HB3	1:A:175:ILE:HD13	1.95	0.49
2:G:635:MET:O	2:G:637:ALA:N	2.39	0.49
1:A:157:ASP:HA	1:A:182:GLY:HA3	1.94	0.48
1:A:192:ILE:HD11	1:A:253:GLU:HB2	1.95	0.48
1:A:44:MET:HG3	1:A:45:VAL:H	1.76	0.48
1:A:44:MET:HG3	1:A:45:VAL:O	2.13	0.48
2:G:425:ILE:H	2:G:425:ILE:HD12	1.78	0.48
2:G:430:LYS:CG	2:G:430:LYS:O	2.60	0.48
2:G:614:PHE:CD1	2:G:614:PHE:C	2.87	0.48
2:G:645:CYS:SG	2:G:673:LEU:CD2	3.01	0.48
1:A:150:GLY:HA2	1:A:293:LEU:HD12	1.96	0.48
2:G:433:VAL:O	2:G:434:ASP:C	2.52	0.48
2:G:452:ASN:O	2:G:453:TYR:O	2.31	0.48
2:G:538:LEU:HD12	2:G:568:VAL:O	2.14	0.48
2:G:730:VAL:CG1	2:G:736:TRP:CG	2.97	0.48
2:G:427:GLY:CA	2:G:526:ARG:HG2	2.43	0.48
2:G:426:GLU:CG	2:G:431:VAL:CG2	2.91	0.48
1:A:282:ILE:O	1:A:290:ARG:HD3	2.13	0.47
2:G:562:ASN:ND2	2:G:731:GLY:O	2.47	0.47
1:A:361:GLU:OE1	1:A:373:LYS:HE3	2.14	0.47
2:G:711:ARG:HA	2:G:711:ARG:HD3	1.61	0.47
1:A:64:ILE:HD12	1:A:64:ILE:H	1.79	0.47
1:A:210:ARG:HG2	1:A:210:ARG:HH11	1.79	0.47
1:A:120:THR:HG23	1:A:132:MET:SD	2.55	0.47
2:G:412:MET:O	2:G:413:ASP:HB2	2.14	0.47
2:G:684:VAL:HG23	2:G:684:VAL:O	2.15	0.47
1:A:178:LEU:HD22	1:A:180:LEU:HB3	1.96	0.47
2:G:558:ALA:O	2:G:560:ALA:N	2.48	0.47
2:G:592:GLN:O	2:G:595:LEU:N	2.47	0.47
2:G:595:LEU:HD11	2:G:602:PRO:HG3	1.90	0.47
2:G:578:TRP:HB2	2:G:614:PHE:HE2	1.80	0.47
1:A:317:ILE:HG22	1:A:327:ILE:HD12	1.96	0.46
1:A:47:MET:N	5:A:2018:HOH:O	2.35	0.46
2:G:455:HIS:CE1	2:G:460:GLY:N	2.83	0.46
1:A:287:ILE:HA	1:A:290:ARG:HG3	1.96	0.46
1:A:141:SER:OG	1:A:338:SER:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:MET:HG2	1:A:209:VAL:HG21	1.98	0.46
2:G:440:GLN:N	2:G:440:GLN:CD	2.69	0.46
2:G:707:ASP:CG	2:G:707:ASP:O	2.54	0.46
1:A:202:THR:HG22	1:A:204:ALA:H	1.81	0.46
2:G:558:ALA:CB	2:G:622:ALA:HA	2.43	0.46
2:G:596:ARG:O	2:G:597:VAL:C	2.54	0.46
2:G:647:ASN:C	2:G:647:ASN:HD22	2.18	0.46
2:G:570:LYS:HG3	2:G:572:PRO:HD3	1.96	0.46
2:G:585:GLU:O	2:G:588:LYS:N	2.49	0.46
1:A:330:ILE:HD12	1:A:330:ILE:H	1.81	0.45
2:G:428:SER:OG	2:G:428:SER:O	2.35	0.45
1:A:73:HIS:CA	1:A:159:VAL:HG13	2.44	0.45
1:A:352:PHE:HE2	1:A:356:TRP:CH2	2.33	0.45
1:A:113:LYS:HB3	1:A:371:HIS:CE1	2.52	0.45
2:G:526:ARG:CG	2:G:526:ARG:NH1	2.59	0.45
1:A:337:TYR:O	1:A:341:ILE:HG13	2.16	0.45
2:G:563:SER:HB3	2:G:631:LYS:HG2	1.99	0.45
2:G:571:THR:O	2:G:571:THR:HG23	2.17	0.45
2:G:564:ASN:CG	2:G:635:MET:HE1	2.37	0.45
2:G:635:MET:C	2:G:637:ALA:H	2.20	0.45
1:A:222:ASP:HB3	1:A:225:ASN:HD22	1.81	0.45
1:A:38:PRO:C	1:A:40:HIS:H	2.19	0.45
2:G:425:ILE:HD11	2:G:448:ILE:CD1	2.46	0.45
2:G:424:ARG:HH22	2:G:524:THR:HG23	1.78	0.45
2:G:635:MET:SD	2:G:732:TRP:HZ3	2.40	0.45
1:A:222:ASP:CG	1:A:225:ASN:ND2	2.70	0.45
1:A:185:LEU:HD21	1:A:261:LEU:HD22	1.99	0.45
2:G:603:VAL:HG12	2:G:603:VAL:O	2.17	0.45
2:G:595:LEU:HD13	2:G:602:PRO:HD3	1.98	0.45
1:A:136:ILE:N	1:A:136:ILE:CD1	2.78	0.44
2:G:415:ASP:CB	2:G:417:THR:HG23	2.48	0.44
2:G:421:GLN:OE1	2:G:422:ILE:N	2.50	0.44
1:A:302:GLY:HA3	4:A:1377:ATP:O4'	2.16	0.44
1:A:203:THR:HA	1:A:206:ARG:HH11	1.82	0.44
2:G:558:ALA:C	2:G:560:ALA:H	2.21	0.44
1:A:55:GLY:O	1:A:56:ASP:C	2.56	0.44
2:G:610:GLU:HG3	2:G:615:TRP:CZ2	2.53	0.44
2:G:422:ILE:HG12	2:G:449:ILE:HB	2.00	0.44
2:G:526:ARG:C	2:G:527:GLU:OE2	2.56	0.44
1:A:202:THR:HG22	1:A:204:ALA:N	2.33	0.44
1:A:324:THR:O	1:A:325:MET:C	2.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:467:GLN:CG	2:G:476:VAL:HG13	2.47	0.44
2:G:707:ASP:CG	2:G:709:ALA:H	2.20	0.44
1:A:329:ILE:O	1:A:329:ILE:HG22	2.17	0.44
2:G:646:SER:HB2	2:G:670:ASP:CG	2.38	0.44
2:G:704:ILE:HG23	2:G:711:ARG:HG3	1.99	0.44
1:A:256:ARG:HG2	1:A:256:ARG:HH11	1.83	0.44
1:A:44:MET:CG	1:A:45:VAL:O	2.66	0.44
1:A:18:LYS:HD3	1:A:18:LYS:N	2.33	0.43
2:G:558:ALA:HA	2:G:618:LEU:HD13	2.00	0.43
1:A:65:LEU:O	1:A:66:THR:CG2	2.59	0.43
2:G:569:LEU:O	2:G:575:ALA:HA	2.18	0.43
1:A:70:PRO:HA	1:A:78:ASN:HB3	2.01	0.43
2:G:565:ASP:HA	2:G:587:GLU:OE1	2.18	0.43
2:G:704:ILE:O	2:G:705:GLU:CB	2.63	0.43
1:A:87:HIS:CD2	1:A:91:TYR:HD1	2.36	0.43
2:G:711:ARG:NH1	2:G:715:THR:HG21	2.34	0.43
1:A:293:LEU:HA	1:A:293:LEU:HD12	1.81	0.43
2:G:526:ARG:HH11	2:G:526:ARG:HG3	1.79	0.43
2:G:705:GLU:C	2:G:707:ASP:N	2.68	0.43
1:A:136:ILE:HD13	5:A:2078:HOH:O	2.18	0.43
1:A:374:CYS:O	1:A:375:PHE:O	2.37	0.43
1:A:62:ARG:NH1	5:A:2025:HOH:O	2.35	0.43
2:G:440:GLN:H	2:G:440:GLN:CD	2.22	0.43
2:G:598:LEU:HA	2:G:598:LEU:HD23	1.64	0.43
1:A:62:ARG:HA	1:A:65:LEU:HD13	2.01	0.42
2:G:412:MET:O	2:G:413:ASP:CB	2.67	0.42
2:G:726:PRO:O	2:G:730:VAL:HG23	2.19	0.42
2:G:437:THR:HB	2:G:440:GLN:HG2	2.01	0.42
1:A:147:ARG:NH2	1:A:330:ILE:HG12	2.35	0.42
1:A:27:PRO:HD3	1:A:340:TRP:CD2	2.54	0.42
2:G:674:LEU:HD12	2:G:729:PHE:CE1	2.54	0.42
1:A:360:GLN:O	1:A:364:GLU:HG3	2.19	0.42
1:A:367:PRO:O	1:A:368:SER:C	2.58	0.42
1:A:312:ARG:NH1	1:A:316:GLU:OE1	2.53	0.42
2:G:677:TRP:O	2:G:711:ARG:NH1	2.53	0.42
1:A:238:LYS:HG2	1:A:254:ARG:NH1	2.35	0.42
1:A:353:GLN:HA	1:A:356:TRP:CD1	2.55	0.42
2:G:554:VAL:HG12	2:G:555:LEU:N	2.35	0.42
2:G:635:MET:SD	2:G:732:TRP:HH2	2.43	0.42
1:A:18:LYS:HG3	1:A:30:VAL:HG22	2.02	0.41
1:A:334:GLU:H	1:A:334:GLU:HG3	1.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:533:PRO:O	2:G:534:ALA:HB2	2.20	0.41
2:G:714:ARG:HA	2:G:714:ARG:HD3	1.43	0.41
1:A:352:PHE:O	1:A:354:GLN:N	2.54	0.41
2:G:577:LEU:CD2	2:G:577:LEU:O	2.69	0.41
1:A:192:ILE:CD1	1:A:253:GLU:CB	2.99	0.41
2:G:435:PRO:HA	2:G:438:TYR:CD2	2.55	0.41
2:G:512:PHE:C	2:G:514:GLY:H	2.24	0.41
2:G:450:LEU:HD12	2:G:451:TYR:N	2.35	0.41
2:G:571:THR:O	2:G:574:ALA:N	2.37	0.41
1:A:193:LEU:CD2	1:A:253:GLU:HG3	2.51	0.41
1:A:210:ARG:NH1	1:A:210:ARG:HG2	2.36	0.41
1:A:54:VAL:CG1	1:A:55:GLY:N	2.83	0.41
2:G:525:SER:CB	5:G:2068:HOH:O	2.60	0.41
2:G:644:ALA:HA	2:G:672:MET:SD	2.61	0.41
1:A:198:TYR:CE2	1:A:248:ILE:HG22	2.56	0.41
2:G:421:GLN:HA	2:G:421:GLN:OE1	2.20	0.41
2:G:424:ARG:HG3	2:G:447:TYR:CZ	2.56	0.41
2:G:578:TRP:CD1	2:G:614:PHE:CZ	3.09	0.41
2:G:543:ALA:HA	2:G:548:ALA:O	2.20	0.40
2:G:569:LEU:HD11	2:G:618:LEU:CD2	2.51	0.40
2:G:632:ASP:CG	2:G:634:LYS:HD2	2.41	0.40
2:G:684:VAL:HG22	2:G:721:LYS:HA	2.02	0.40
2:G:707:ASP:HB2	2:G:711:ARG:HB2	1.92	0.40
1:A:123:MET:HG3	1:A:132:MET:CE	2.51	0.40
1:A:285:CYS:O	1:A:290:ARG:NH1	2.54	0.40
2:G:713:ARG:HG2	5:G:2136:HOH:O	2.20	0.40
1:A:303:THR:O	1:A:303:THR:HG22	2.21	0.40
1:A:352:PHE:HD2	1:A:356:TRP:CZ2	2.38	0.40
1:A:352:PHE:CE1	1:A:355:MET:HE2	2.56	0.40
2:G:585:GLU:HA	2:G:588:LYS:HD3	2.04	0.40
2:G:642:LEU:HB3	2:G:657:VAL:HB	2.03	0.40
1:A:295:ALA:HA	1:A:328:LYS:HB2	2.03	0.40
2:G:464:TYR:CZ	2:G:508:LEU:HB2	2.56	0.40
2:G:673:LEU:HD13	2:G:673:LEU:HA	1.98	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:MET:SD	5:G:2040:HOH:O[3_655]	1.09	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:MET:CE	2:G:452:ASN:OD1[3_655]	1.40	0.80
5:A:2018:HOH:O	5:G:2040:HOH:O[3_655]	1.86	0.34

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	364/375 (97%)	315 (86%)	37 (10%)	12 (3%)	4	21
2	G	323/331 (98%)	252 (78%)	39 (12%)	32 (10%)	0	2
All	All	687/706 (97%)	567 (82%)	76 (11%)	44 (6%)	1	7

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	SER
2	G	453	TYR
2	G	526	ARG
2	G	534	ALA
2	G	535	SER
2	G	572	PRO
2	G	573	SER
2	G	599	ARG
2	G	600	ALA
2	G	602	PRO
2	G	603	VAL
2	G	621	LYS
2	G	622	ALA
2	G	708	PRO
2	G	709	ALA
1	A	60	SER
1	A	66	THR
1	A	325	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	413	ASP
2	G	536	THR
2	G	559	GLY
2	G	623	ALA
2	G	712	ASP
1	A	62	ARG
1	A	65	LEU
1	A	67	LEU
1	A	182	GLY
2	G	528	GLY
2	G	575	ALA
2	G	604	GLN
2	G	611	PRO
2	G	620	GLY
2	G	738	ASP
1	A	323	SER
1	A	353	GLN
2	G	513	GLY
2	G	533	PRO
2	G	597	VAL
1	A	45	VAL
2	G	636	ASP
2	G	425	ILE
1	A	38	PRO
2	G	735	GLY
2	G	432	PRO

5.3.2 Protein sidechains ⓘ

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	311/318 (98%)	272 (88%)	39 (12%)	4	20
2	G	263/265 (99%)	226 (86%)	37 (14%)	3	16
All	All	574/583 (98%)	498 (87%)	76 (13%)	4	18

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	CYS
1	A	25	ASP
1	A	28	ARG
1	A	33	SER
1	A	38	PRO
1	A	39	ARG
1	A	50	LYS
1	A	51	ASP
1	A	53	TYR
1	A	62	ARG
1	A	64	ILE
1	A	67	LEU
1	A	75	ILE
1	A	84	LYS
1	A	104	LEU
1	A	120	THR
1	A	129	VAL
1	A	178	LEU
1	A	180	LEU
1	A	184	ASP
1	A	185	LEU
1	A	203	THR
1	A	221	LEU
1	A	227	MET
1	A	235	SER
1	A	249	THR
1	A	250	ILE
1	A	253	GLU
1	A	261	LEU
1	A	265	SER
1	A	284	LYS
1	A	286	ASP
1	A	287	ILE
1	A	293	LEU
1	A	300	SER
1	A	312	ARG
1	A	334	GLU
1	A	354	GLN
1	A	368	SER
2	G	419	GLN
2	G	421	GLN
2	G	424	ARG
2	G	440	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	449	ILE
2	G	450	LEU
2	G	454	ARG
2	G	470	GLN
2	G	472	THR
2	G	526	ARG
2	G	527	GLU
2	G	531	THR
2	G	533	PRO
2	G	542	ARG
2	G	562	ASN
2	G	569	LEU
2	G	572	PRO
2	G	573	SER
2	G	589	THR
2	G	594	LEU
2	G	605	VAL
2	G	611	PRO
2	G	614	PHE
2	G	647	ASN
2	G	651	ARG
2	G	668	THR
2	G	669	ASP
2	G	673	LEU
2	G	674	LEU
2	G	682	VAL
2	G	707	ASP
2	G	711	ARG
2	G	713	ARG
2	G	714	ARG
2	G	715	THR
2	G	730	VAL
2	G	738	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	92	ASN
1	A	128	ASN
1	A	137	GLN
1	A	225	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	280	ASN
2	G	440	GLN
2	G	452	ASN
2	G	455	HIS
2	G	461	GLN
2	G	540	GLN
2	G	592	GLN
2	G	601	GLN
2	G	604	GLN
2	G	647	ASN
2	G	689	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	A	1377	3	26,33,33	1.43	5 (19%)	31,52,52	3.90	10 (32%)

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
4	ATP	A	1377	3	-	5/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1377	ATP	C2'-C1'	-3.73	1.48	1.53
4	A	1377	ATP	C5-C4	2.86	1.48	1.40
4	A	1377	ATP	C2-N3	2.50	1.36	1.32
4	A	1377	ATP	C5-N7	-2.26	1.31	1.39
4	A	1377	ATP	O4'-C4'	-2.08	1.40	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1377	ATP	C2-N1-C6	13.96	142.64	118.75
4	A	1377	ATP	N3-C2-N1	-11.16	111.23	128.68
4	A	1377	ATP	C5-C6-N1	-6.21	106.28	120.35
4	A	1377	ATP	C5-C6-N6	4.29	126.87	120.35
4	A	1377	ATP	PB-O3B-PG	-4.23	118.31	132.83
4	A	1377	ATP	N6-C6-N1	3.99	126.85	118.57
4	A	1377	ATP	O3G-PG-O2G	3.96	122.79	107.64
4	A	1377	ATP	PA-O3A-PB	-3.90	119.46	132.83
4	A	1377	ATP	O4'-C1'-C2'	-2.26	103.62	106.93
4	A	1377	ATP	O2B-PB-O1B	2.18	123.02	112.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

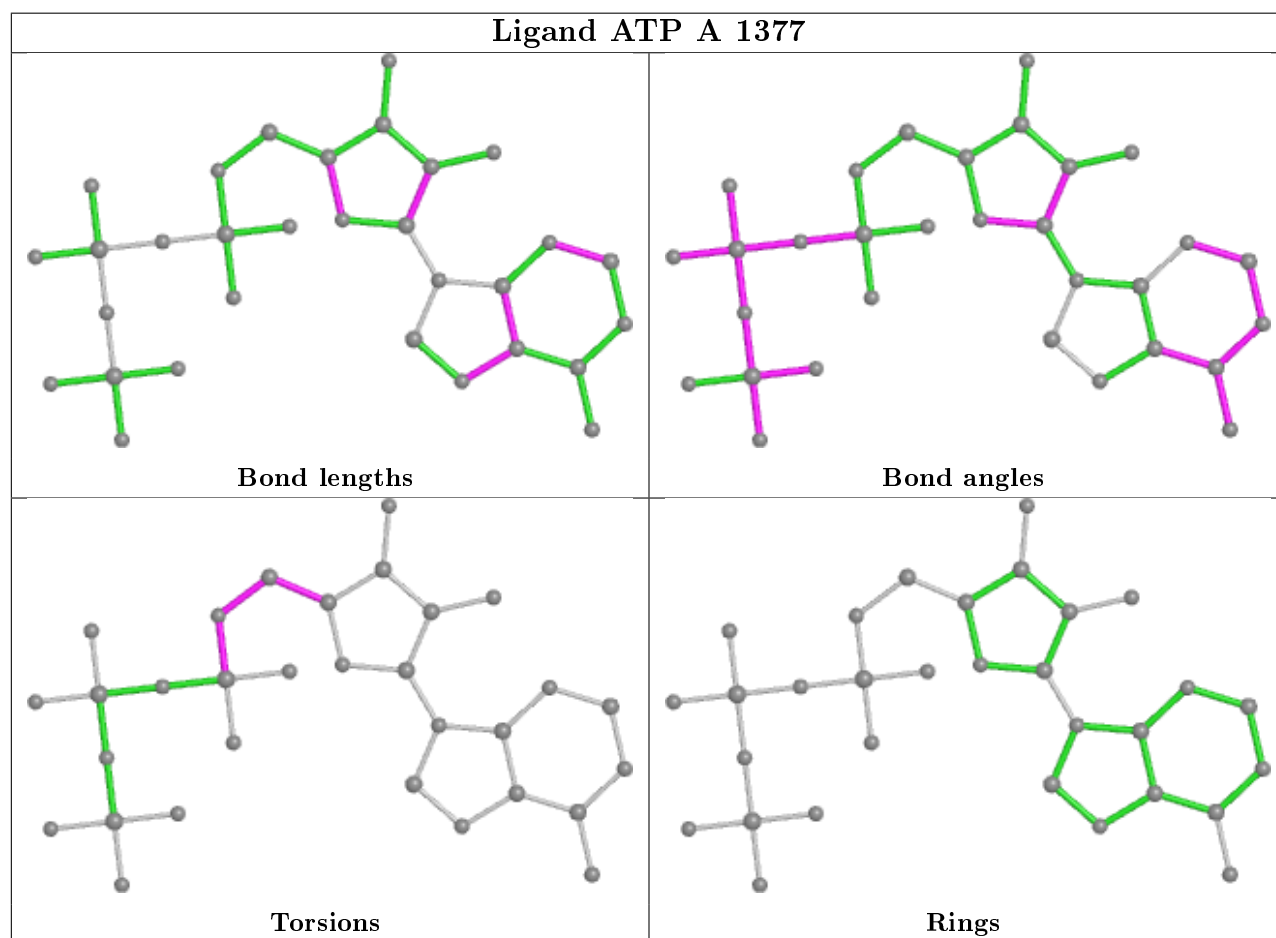
Mol	Chain	Res	Type	Atoms
4	A	1377	ATP	C5'-O5'-PA-O1A
4	A	1377	ATP	C5'-O5'-PA-O2A
4	A	1377	ATP	C5'-O5'-PA-O3A
4	A	1377	ATP	C3'-C4'-C5'-O5'
4	A	1377	ATP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1377	ATP	1	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 than 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

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	368/375 (98%)	-0.38	9 (2%) 59 30	3, 18, 77, 97	0
2	G	327/331 (98%)	0.02	17 (5%) 27 10	8, 32, 69, 83	0
All	All	695/706 (98%)	-0.19	26 (3%) 41 17	3, 22, 70, 97	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	PRO	5.6
2	G	712	ASP	4.1
2	G	635	MET	3.6
1	A	39	ARG	3.3
2	G	413	ASP	3.3
1	A	53	TYR	3.0
2	G	597	VAL	3.0
1	A	66	THR	3.0
2	G	713	ARG	3.0
2	G	412	MET	2.9
2	G	526	ARG	2.9
2	G	709	ALA	2.7
1	A	5	THR	2.5
2	G	598	LEU	2.5
2	G	572	PRO	2.4
1	A	36	GLY	2.3
2	G	573	SER	2.3
1	A	52	SER	2.3
1	A	40	HIS	2.3
2	G	528	GLY	2.2
2	G	710	ASN	2.2
2	G	527	GLU	2.2
1	A	62	ARG	2.2
2	G	708	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	455	HIS	2.1
2	G	620	GLY	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](#)

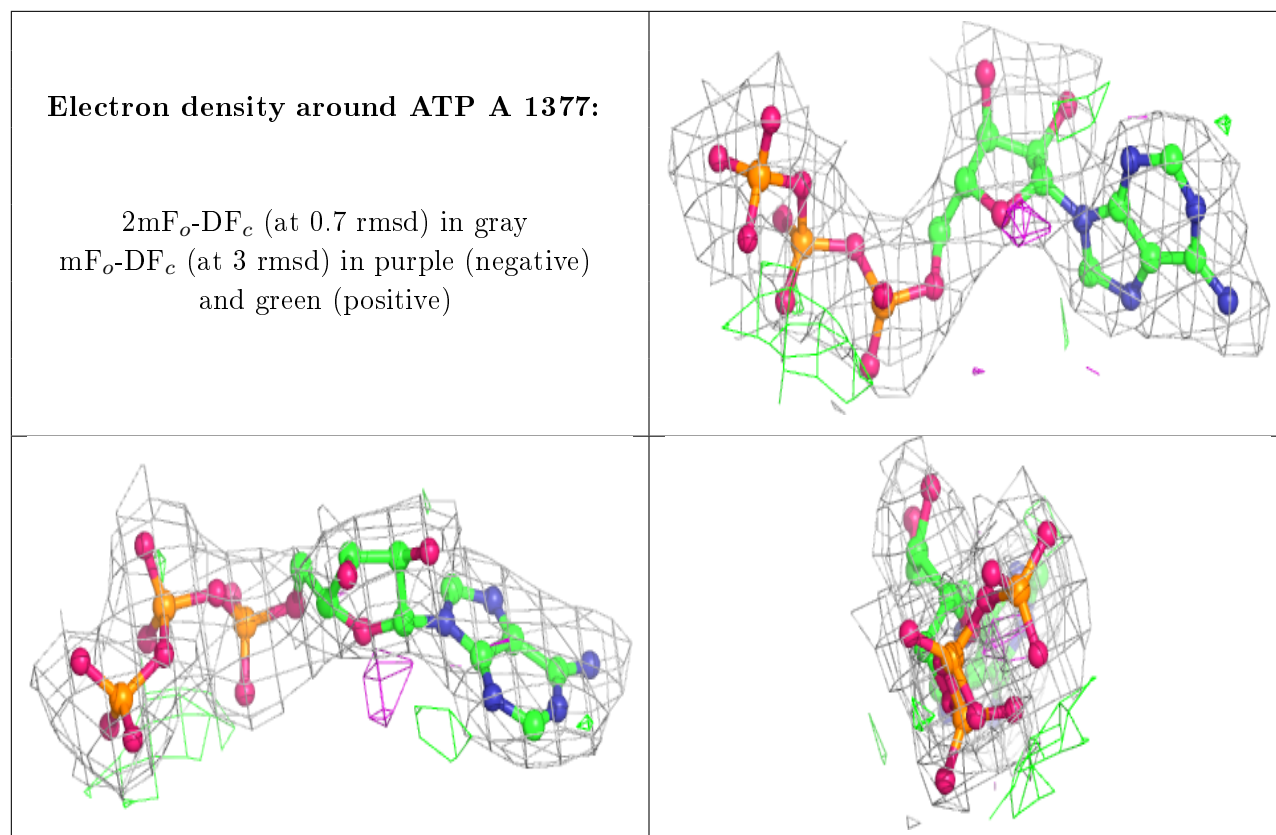
There are no carbohydrates in this entry.

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. 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(\AA^2)	Q<0.9
3	CA	G	1744	1/1	0.94	0.08	23,23,23,23	0
4	ATP	A	1377	31/31	0.97	0.11	2,4,6,7	0
3	CA	A	1376	1/1	0.97	0.17	28,28,28,28	0
3	CA	G	1746	1/1	0.97	0.08	15,15,15,15	0
3	CA	G	1745	1/1	0.97	0.07	29,29,29,29	0
3	CA	G	1743	1/1	0.99	0.08	15,15,15,15	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 ⓘ

There are no such residues in this entry.