



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:53 PM UTC

PDB ID : 3FFK / pdb_00003ffk
Title : Crystal structure of human Gelsolin domains G1-G3 bound to Actin
Authors : Chumnarnsilpa, S.; Robinson, R.C.; Burtnick, L.D.
Deposited on : 2008-12-03
Resolution : 3.00 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

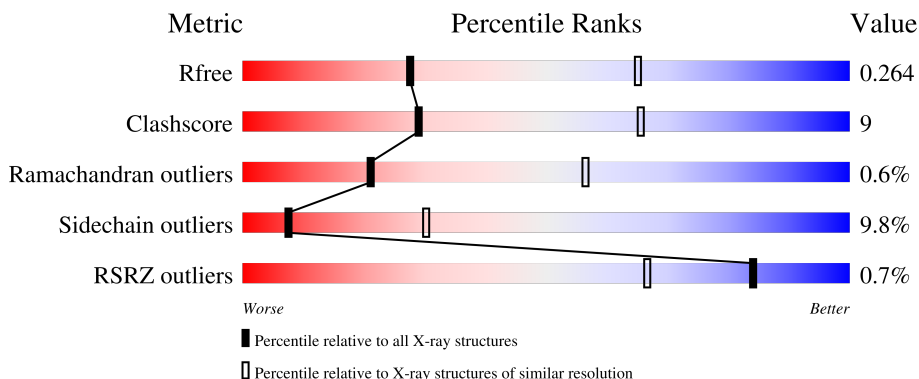
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	377	 73% 17% • 8%
1	D	377	 70% 19% •• 8%
2	B	377	 75% 19% ••
2	E	377	 71% 20% • 6%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11677 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 plasma gelsolin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	Total	C	N	O	S	0	4	0
			2770	1754	491	518	7			
1	D	346	Total	C	N	O	S	0	1	0
			2737	1734	483	513	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP P06396
A	24	PRO	-	expression tag	UNP P06396
D	23	GLY	-	expression tag	UNP P06396
D	24	PRO	-	expression tag	UNP P06396

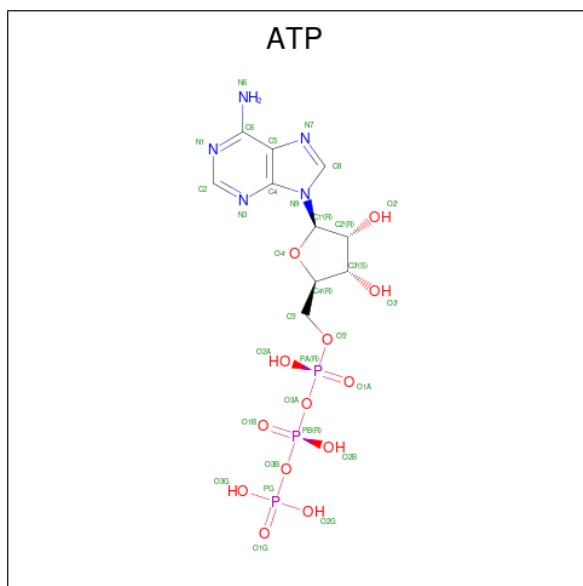
- Molecule 2 is a protein called actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	365	Total	C	N	O	S	0	0	0
			2846	1801	477	548	20			
2	E	355	Total	C	N	O	S	0	1	0
			2779	1763	462	536	18			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		
3	B	1	Total	Ca	0	0
			1	1		
3	D	4	Total	Ca	0	0
			4	4		
3	E	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

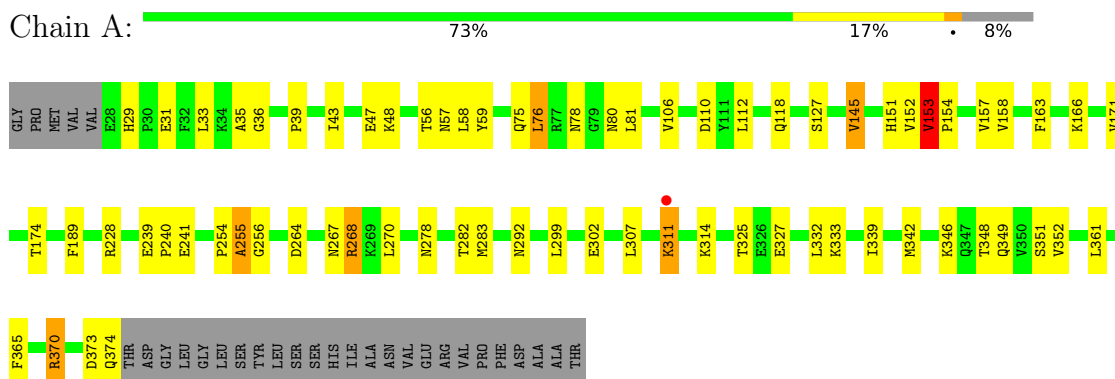
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total	O	0	0
			130	130		
5	B	114	Total	O	0	0
			114	114		
5	D	103	Total	O	0	0
			103	103		
5	E	126	Total	O	0	0
			126	126		

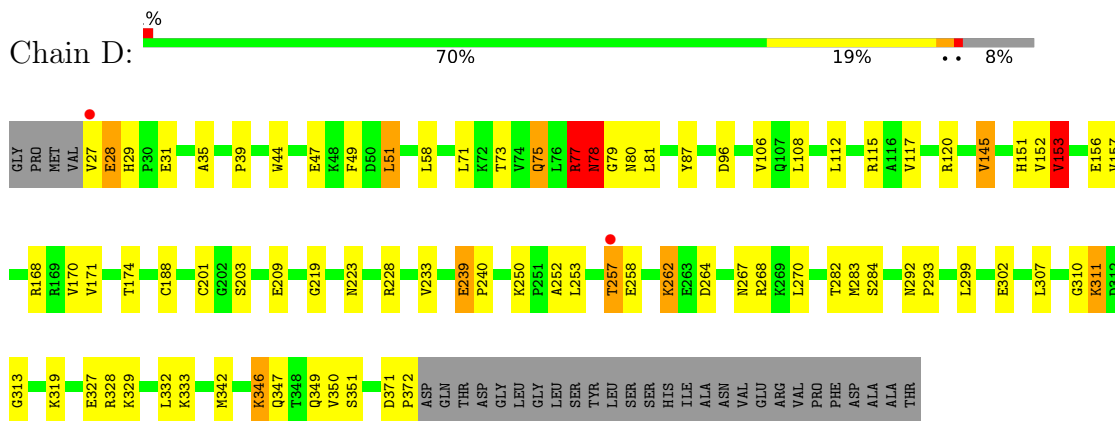
3 Residue-property plots [i](#)

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.

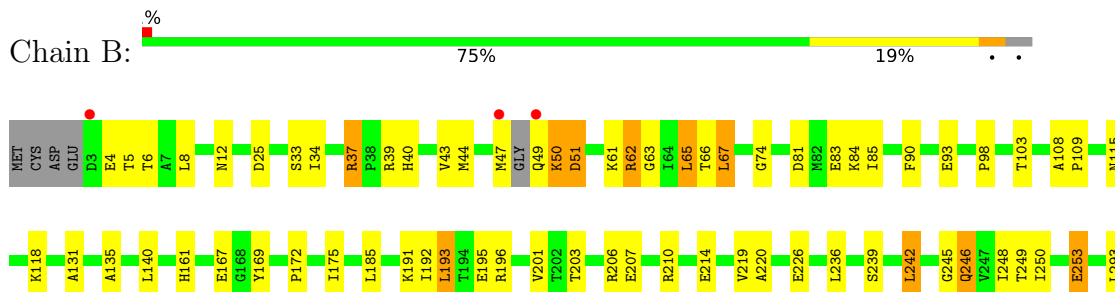
- Molecule 1: plasma gelsolin



- Molecule 1: plasma gelsolin

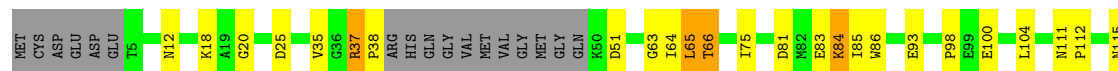


- Molecule 2: actin, alpha skeletal muscle





- Molecule 2: actin, alpha skeletal muscle



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.18Å 146.92Å 148.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.00) 99.6 (30.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 3.00Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.273 0.196 , 0.264	Depositor DCC
R_{free} test set	2264 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtrriage
Anisotropy	0.028	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.007 for -h,l,k	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11677	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 [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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/2841	0.88	3/3834 (0.1%)
1	D	0.54	1/2802 (0.0%)	0.85	3/3785 (0.1%)
2	B	0.57	0/2906	0.89	1/3938 (0.0%)
2	E	0.58	0/2838	0.90	1/3849 (0.0%)
All	All	0.56	1/11387 (0.0%)	0.88	8/15406 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	153	VAL	CA-CB	5.59	1.59	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	THR	N-CA-C	6.56	119.54	110.35
1	A	255	ALA	N-CA-C	6.13	117.07	108.00
1	A	153	VAL	CA-C-N	5.57	125.89	119.93
1	A	153	VAL	C-N-CA	5.57	125.89	119.93
1	D	78	ASN	N-CA-C	5.35	125.98	111.00
2	E	235	SER	N-CA-C	-5.31	107.46	114.04
1	D	77	ARG	CA-C-N	5.10	130.88	121.70
1	D	77	ARG	C-N-CA	5.10	130.88	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2770	0	2730	45	0
1	D	2737	0	2691	47	0
2	B	2846	0	2808	53	0
2	E	2779	0	2749	59	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
3	D	4	0	0	0	0
3	E	1	0	0	0	0
4	B	31	0	12	0	0
4	E	31	0	12	1	0
5	A	130	0	0	1	0
5	B	114	0	0	2	0
5	D	103	0	0	2	0
5	E	126	0	0	7	0
All	All	11677	0	11002	193	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 9.

All (193) 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:255:ALA:CB	1:A:256:GLY:HA2	1.54	1.35
1:A:255:ALA:HB1	1:A:256:GLY:CA	1.71	1.18
1:D:311:LYS:H	1:D:311:LYS:HD2	1.04	1.11
2:B:245:GLY:CA	2:B:246:GLN:HB3	1.89	1.01
1:D:151:HIS:HD2	2:E:25:ASP:OD1	1.47	0.95
1:A:292:ASN:HD21	1:A:365:PHE:HD2	1.13	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ARG:HH11	2:B:37:ARG:HG2	1.33	0.92
1:D:311:LYS:H	1:D:311:LYS:CD	1.82	0.92
2:B:245:GLY:HA3	2:B:246:GLN:HB3	1.50	0.89
1:D:311:LYS:HD2	1:D:311:LYS:N	1.88	0.89
2:E:37:ARG:HG2	2:E:37:ARG:HH11	1.39	0.88
1:D:283:MET:HE1	1:D:327:GLU:HA	1.56	0.87
1:A:311[B]:LYS:H	1:A:311[B]:LYS:HD2	1.39	0.86
1:D:77:ARG:HA	1:D:79:GLY:N	1.95	0.82
1:D:153:VAL:HG22	1:D:156:GLU:HB2	1.62	0.82
1:A:118:GLN:CD	2:B:167:GLU:HG3	2.04	0.81
1:A:374:GLN:HG2	2:B:51:ASP:HB3	1.62	0.80
2:B:245:GLY:CA	2:B:246:GLN:CB	2.59	0.79
1:A:346[B]:LYS:HA	1:A:348:THR:H	1.47	0.78
2:B:245:GLY:HA2	2:B:246:GLN:HB3	1.64	0.78
1:D:262:LYS:HB3	1:D:262:LYS:NZ	1.97	0.77
2:E:37:ARG:HH11	2:E:37:ARG:CG	1.97	0.77
1:D:151:HIS:CD2	2:E:25:ASP:OD1	2.35	0.76
1:A:346[A]:LYS:HA	1:A:348:THR:H	1.48	0.75
1:A:267:ASN:HA	1:A:270:LEU:HG	1.69	0.72
1:A:151:HIS:CD2	2:B:25:ASP:OD1	2.44	0.71
1:A:255:ALA:CB	1:A:256:GLY:CA	2.41	0.70
1:A:255:ALA:HB1	1:A:256:GLY:HA2	0.76	0.70
2:B:49:GLN:HG3	2:B:50:LYS:H	1.54	0.70
1:D:188:CYS:HG	1:D:201:CYS:HG	0.74	0.70
1:A:311[B]:LYS:H	1:A:311[B]:LYS:CD	1.99	0.69
2:B:210:ARG:O	2:B:214:GLU:HG2	1.92	0.69
2:E:270:GLU:OE2	2:E:270:GLU:HA	1.91	0.69
1:D:257:THR:HG22	1:D:258:GLU:H	1.56	0.69
2:E:196:ARG:NH2	2:E:249:THR:O	2.27	0.68
1:D:319:LYS:HD2	1:D:328:ARG:HG2	1.76	0.68
2:E:304:THR:O	2:E:335:ARG:NH1	2.27	0.68
2:E:38:PRO:HD3	2:E:51:ASP:O	1.94	0.67
1:A:76:LEU:HB2	1:A:80:ASN:O	1.95	0.67
2:B:245:GLY:HA2	2:B:246:GLN:CB	2.23	0.67
2:E:205:GLU:HA	2:E:208:ILE:HD12	1.78	0.66
1:A:29:HIS:CD2	1:A:31:GLU:H	2.14	0.65
2:B:353:GLN:HB2	5:B:378:HOH:O	1.96	0.65
2:B:352:PHE:HE2	2:B:356:TRP:CH2	2.15	0.65
1:D:29:HIS:CD2	1:D:31:GLU:H	2.15	0.64
1:D:311:LYS:CD	1:D:311:LYS:N	2.54	0.64
1:D:44:TRP:CB	1:D:51:LEU:HD22	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:VAL:CG1	2:B:312:ARG:HG3	2.30	0.62
1:D:219:GLY:O	1:D:223:ASN:HB3	2.00	0.62
2:E:210:ARG:O	2:E:214:GLU:HG2	1.99	0.61
2:E:131:ALA:HB1	2:E:356:TRP:HB3	1.82	0.61
2:E:213:LYS:O	2:E:217:CYS:HB2	2.00	0.61
2:E:352:PHE:HE2	2:E:356:TRP:CZ3	2.18	0.61
1:D:44:TRP:HB3	1:D:51:LEU:HD22	1.83	0.61
2:B:39:ARG:HB3	2:B:66:THR:HG23	1.83	0.61
2:E:12:ASN:HD21	2:E:86:TRP:HE1	1.49	0.60
1:A:268:ARG:HD3	1:A:292:ASN:O	2.02	0.60
2:E:190:MET:HG3	2:E:209:VAL:HG21	1.83	0.59
1:D:77:ARG:HA	1:D:78:ASN:C	2.26	0.59
2:B:135:ALA:HB3	2:B:140:LEU:HD11	1.83	0.59
2:B:131:ALA:HB1	2:B:356:TRP:HB3	1.85	0.59
2:E:250:ILE:HG13	2:E:253:GLU:HG2	1.85	0.58
1:A:311[B]:LYS:HD2	1:A:311[B]:LYS:N	2.16	0.58
1:A:268:ARG:CD	1:A:292:ASN:O	2.52	0.58
2:B:37:ARG:HG2	2:B:37:ARG:NH1	2.11	0.57
1:A:283:MET:HE1	1:A:327:GLU:HA	1.86	0.57
1:D:47:GLU:HG2	1:D:145:VAL:HG11	1.85	0.57
2:E:66:THR:HA	5:E:478:HOH:O	2.05	0.56
1:D:27:VAL:HG23	1:D:28:GLU:H	1.69	0.56
1:D:262:LYS:HB3	1:D:262:LYS:HZ3	1.69	0.55
2:E:51:ASP:HB3	5:E:418:HOH:O	2.07	0.55
1:D:346:LYS:O	1:D:347:GLN:HB2	2.05	0.55
2:B:219:VAL:HG12	2:B:312:ARG:HG3	1.89	0.54
2:E:352:PHE:CE2	2:E:356:TRP:CZ3	2.96	0.54
2:E:190:MET:HG2	2:E:200:PHE:HB3	1.89	0.54
2:B:37:ARG:HH11	2:B:37:ARG:CG	2.11	0.54
1:A:346[B]:LYS:HA	1:A:348:THR:N	2.20	0.54
2:E:220:ALA:HB1	2:E:226:GLU:HG3	1.89	0.54
2:E:12:ASN:ND2	2:E:86:TRP:HE1	2.06	0.53
1:D:283:MET:CE	1:D:327:GLU:HA	2.34	0.53
1:A:346[A]:LYS:HA	1:A:348:THR:N	2.20	0.53
1:D:329:LYS:HE2	5:D:798:HOH:O	2.08	0.53
2:E:65:LEU:O	5:E:478:HOH:O	2.19	0.53
1:D:228:ARG:NH2	2:E:93:GLU:OE1	2.42	0.53
1:D:39:PRO:HA	1:D:73:THR:O	2.09	0.52
1:D:171:VAL:HG11	1:D:209:GLU:HA	1.91	0.52
2:E:253:GLU:HA	2:E:256:ARG:HB2	1.91	0.52
2:E:218:TYR:O	2:E:255:PHE:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:ARG:HD2	1:D:292:ASN:O	2.10	0.50
1:D:292:ASN:HB2	1:D:293:PRO:HA	1.92	0.50
2:B:34:ILE:HD12	2:B:67:LEU:HG	1.94	0.49
2:B:61:LYS:HB3	2:B:65:LEU:HD21	1.94	0.49
1:D:35:ALA:HB1	1:D:71:LEU:HD23	1.94	0.49
2:E:322:PRO:O	2:E:324:THR:N	2.45	0.49
1:A:374:GLN:HA	2:B:51:ASP:HB3	1.94	0.48
1:D:170:VAL:HG21	1:D:268:ARG:HD3	1.94	0.48
2:E:250:ILE:HG13	2:E:253:GLU:CG	2.43	0.48
2:B:90:PHE:HB3	2:B:98:PRO:HG3	1.95	0.48
1:A:373:ASP:O	1:A:374:GLN:HG3	2.13	0.48
2:B:62:ARG:HG3	2:B:63:GLY:N	2.28	0.48
2:B:304:THR:O	2:B:335:ARG:NH1	2.46	0.48
1:A:110:ASP:OD2	2:B:169:TYR:OH	2.28	0.48
2:B:196:ARG:NH1	2:B:253:GLU:OE1	2.46	0.48
2:B:220:ALA:HB1	2:B:226:GLU:HG3	1.96	0.47
1:D:87:TYR:CE1	1:D:120:ARG:HG3	2.50	0.47
1:D:262:LYS:HB3	1:D:262:LYS:HZ2	1.77	0.47
2:E:347:ALA:HA	2:E:352:PHE:CD2	2.49	0.47
1:A:39:PRO:HG3	1:A:75:GLN:HB2	1.96	0.47
2:E:332:PRO:O	2:E:335:ARG:HB3	2.15	0.47
2:B:352:PHE:CE2	2:B:356:TRP:CH2	3.00	0.47
2:B:362:TYR:C	2:B:364:GLU:H	2.22	0.47
2:B:356:TRP:CD1	5:B:410:HOH:O	2.67	0.47
2:B:297:ASN:HB2	2:B:328:LYS:O	2.13	0.47
1:D:267:ASN:HA	1:D:270:LEU:HG	1.96	0.46
1:A:29:HIS:CD2	1:A:31:GLU:HB2	2.51	0.46
2:E:116:ARG:HA	2:E:119:MET:HE3	1.96	0.46
2:E:222:ASP:OD1	2:E:222:ASP:C	2.59	0.46
1:D:239:GLU:HA	1:D:240:PRO:HD3	1.77	0.46
1:D:371:ASP:HA	1:D:372:PRO:HD2	1.69	0.46
2:E:219:VAL:CG1	2:E:312:ARG:HG3	2.46	0.46
2:E:51:ASP:CB	5:E:418:HOH:O	2.63	0.46
1:D:44:TRP:HB2	1:D:51:LEU:HD22	1.97	0.46
2:E:222:ASP:CG	2:E:225:ASN:HD22	2.24	0.46
2:B:49:GLN:CG	2:B:50:LYS:H	2.21	0.46
1:A:47:GLU:O	1:A:48:LYS:C	2.59	0.45
1:D:311:LYS:HB3	5:D:853:HOH:O	2.15	0.45
2:E:303:THR:O	2:E:303:THR:HG22	2.17	0.45
1:A:57:ASN:ND2	5:A:792:HOH:O	2.50	0.45
2:E:195:GLU:HG2	5:E:393:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:PRO:HA	2:B:175:ILE:HD12	1.99	0.45
2:B:193:LEU:HD11	2:B:250:ILE:HD12	1.99	0.45
1:D:252:ALA:O	1:D:253:LEU:HD12	2.17	0.44
1:A:151:HIS:HD2	2:B:25:ASP:OD1	1.96	0.44
2:B:207:GLU:OE1	2:B:210:ARG:NH1	2.50	0.44
2:E:35:VAL:HG11	2:E:84:LYS:HD2	1.99	0.44
2:B:8:LEU:HB2	2:B:103:THR:HG23	1.99	0.44
1:A:339:ILE:HG21	1:A:346[B]:LYS:HE2	2.00	0.44
2:B:37:ARG:NH2	2:B:81:ASP:OD1	2.44	0.44
2:E:81:ASP:HA	2:E:84:LYS:HG2	2.00	0.44
2:E:366:GLY:O	2:E:369:ILE:HG22	2.17	0.44
2:E:98:PRO:C	2:E:100:GLU:H	2.25	0.44
1:A:283:MET:HE1	1:A:327:GLU:HG3	1.99	0.43
2:B:226:GLU:OE1	2:B:236:LEU:HD21	2.18	0.43
1:A:370:ARG:HE	1:A:370:ARG:HB2	1.66	0.43
2:B:74:GLY:O	2:B:108:ALA:HB2	2.19	0.43
1:D:39:PRO:HG3	1:D:75:GLN:HB2	2.00	0.43
2:E:214:GLU:HB2	4:E:380:ATP:C6	2.53	0.43
1:A:239:GLU:HA	1:A:240:PRO:HD3	1.81	0.43
1:D:328:ARG:HD3	2:E:100:GLU:OE1	2.18	0.43
2:E:192:ILE:HD12	2:E:192:ILE:HA	1.79	0.43
1:A:268:ARG:HD2	1:A:292:ASN:O	2.19	0.43
2:E:203:THR:HG22	2:E:206:ARG:NH2	2.34	0.43
2:E:353[B]:GLN:HA	2:E:356:TRP:NE1	2.34	0.43
1:A:35:ALA:HA	1:A:36:GLY:HA2	1.81	0.42
1:A:228:ARG:NH2	2:B:93:GLU:OE1	2.51	0.42
1:D:115:ARG:HH11	1:D:115:ARG:HG3	1.84	0.42
1:D:310:GLY:C	1:D:313:GLY:H	2.27	0.42
1:A:166:LYS:C	1:A:171:VAL:HG13	2.44	0.42
2:E:274:ILE:HD12	2:E:313:MET:HE2	2.01	0.42
1:A:43:ILE:HD12	1:A:59:TYR:CG	2.54	0.42
2:B:203:THR:HG22	2:B:206:ARG:HH21	1.84	0.42
2:E:104:LEU:HD11	2:E:346:LEU:HD23	2.01	0.42
2:B:242:LEU:HD12	2:B:246:GLN:O	2.20	0.42
1:D:371:ASP:N	1:D:371:ASP:OD1	2.53	0.42
2:B:40:HIS:HD2	2:B:44:MET:HE3	1.85	0.42
1:A:153:VAL:HA	1:A:154:PRO:HD3	1.90	0.42
2:B:37:ARG:NH1	2:B:37:ARG:CG	2.73	0.42
2:E:350:SER:O	2:E:353[B]:GLN:HG2	2.20	0.42
1:A:163:PHE:O	1:A:189:PHE:HA	2.20	0.42
2:B:318:THR:HA	2:B:327:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:156:GLY:O	2:E:181:ALA:HB1	2.20	0.42
1:A:314:LYS:HE3	1:A:361:LEU:HD13	2.01	0.41
2:B:109:PRO:HG2	2:B:161:HIS:CD2	2.54	0.41
2:E:20:GLY:HA3	5:E:423:HOH:O	2.19	0.41
1:A:292:ASN:ND2	1:A:365:PHE:HD2	1.95	0.41
2:B:192:ILE:CG2	2:B:253:GLU:HB3	2.50	0.41
2:E:37:ARG:CG	2:E:37:ARG:NH1	2.65	0.41
1:A:47:GLU:HG2	1:A:145:VAL:HG11	2.01	0.41
2:E:119:MET:HE3	2:E:119:MET:HB2	1.94	0.41
1:D:49:PHE:CE2	1:D:96:ASP:HB2	2.56	0.41
1:D:168:ARG:HB3	1:D:264:ASP:OD2	2.21	0.41
2:E:180:LEU:HD11	2:E:260:THR:HG22	2.03	0.41
2:E:345:ILE:O	2:E:346:LEU:C	2.63	0.41
1:A:76:LEU:HB3	1:A:78:ASN:ND2	2.36	0.41
2:B:191:LYS:O	2:B:195:GLU:HG3	2.21	0.41
1:A:278:ASN:HB3	1:A:283:MET:HE2	2.03	0.41
1:D:29:HIS:HD2	1:D:31:GLU:H	1.66	0.41
2:E:111:ASN:HA	2:E:112:PRO:HD3	1.94	0.41
2:E:257:CYS:HB3	2:E:258:PRO:HD3	2.02	0.41
2:B:305:MET:HA	2:B:335:ARG:NH1	2.37	0.40
2:E:219:VAL:HG12	2:E:312:ARG:HG3	2.03	0.40
2:B:242:LEU:HD11	2:B:248:ILE:HG23	2.03	0.40
2:E:323:SER:HA	5:E:383:HOH:O	2.20	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	349/377 (93%)	330 (95%)	19 (5%)	0	100 100
1	D	345/377 (92%)	320 (93%)	23 (7%)	2 (1%)	21 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	361/377 (96%)	344 (95%)	13 (4%)	4 (1%)	11	43
2	E	352/377 (93%)	334 (95%)	15 (4%)	3 (1%)	14	48
All	All	1407/1508 (93%)	1328 (94%)	70 (5%)	9 (1%)	21	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	367	PRO
1	D	28	GLU
1	D	78	ASN
2	E	323	SER
2	E	182	GLY
2	B	363	ASP
2	B	50	LYS
2	B	246	GLN
2	E	63	GLY

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	294/314 (94%)	263 (90%)	31 (10%)	6	27
1	D	290/314 (92%)	256 (88%)	34 (12%)	5	23
2	B	308/320 (96%)	282 (92%)	26 (8%)	10	37
2	E	302/320 (94%)	274 (91%)	28 (9%)	8	32
All	All	1194/1268 (94%)	1075 (90%)	119 (10%)	7	29

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	56	THR
1	A	58	LEU

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Mol	Chain	Res	Type
1	A	76	LEU
1	A	81	LEU
1	A	106	VAL
1	A	112	LEU
1	A	127	SER
1	A	145	VAL
1	A	152	VAL
1	A	153	VAL
1	A	157	VAL
1	A	158	VAL
1	A	174	THR
1	A	241	GLU
1	A	264	ASP
1	A	268	ARG
1	A	282	THR
1	A	299	LEU
1	A	302	GLU
1	A	307	LEU
1	A	311[A]	LYS
1	A	311[B]	LYS
1	A	325	THR
1	A	332	LEU
1	A	333	LYS
1	A	342	MET
1	A	349	GLN
1	A	351	SER
1	A	352	VAL
1	A	370	ARG
2	B	4	GLU
2	B	6	THR
2	B	12	ASN
2	B	33	SER
2	B	37	ARG
2	B	43	VAL
2	B	47	MET
2	B	51	ASP
2	B	62	ARG
2	B	65	LEU
2	B	67	LEU
2	B	83	GLU
2	B	84	LYS
2	B	85	ILE

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Mol	Chain	Res	Type
2	B	115	ASN
2	B	118	LYS
2	B	185	LEU
2	B	193	LEU
2	B	201	VAL
2	B	239	SER
2	B	242	LEU
2	B	249	THR
2	B	253	GLU
2	B	293	LEU
2	B	312	ARG
2	B	328	LYS
1	D	51	LEU
1	D	58	LEU
1	D	75	GLN
1	D	77	ARG
1	D	80	ASN
1	D	81	LEU
1	D	106	VAL
1	D	108	LEU
1	D	112	LEU
1	D	117	VAL
1	D	145	VAL
1	D	152	VAL
1	D	153	VAL
1	D	157	VAL
1	D	174	THR
1	D	203	SER
1	D	233	VAL
1	D	239	GLU
1	D	250	LYS
1	D	257	THR
1	D	262	LYS
1	D	282	THR
1	D	284	SER
1	D	299	LEU
1	D	302	GLU
1	D	307	LEU
1	D	311	LYS
1	D	332	LEU
1	D	333	LYS
1	D	342	MET

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Mol	Chain	Res	Type
1	D	346	LYS
1	D	349	GLN
1	D	350	VAL
1	D	351	SER
2	E	18	LYS
2	E	37	ARG
2	E	64	ILE
2	E	65	LEU
2	E	66	THR
2	E	75	ILE
2	E	83	GLU
2	E	84	LYS
2	E	85	ILE
2	E	115	ASN
2	E	185	LEU
2	E	190	MET
2	E	192	ILE
2	E	193	LEU
2	E	195	GLU
2	E	196	ARG
2	E	236	LEU
2	E	244	ASP
2	E	250	ILE
2	E	253	GLU
2	E	271	SER
2	E	293	LEU
2	E	297	ASN
2	E	312	ARG
2	E	335	ARG
2	E	353[A]	GLN
2	E	353[B]	GLN
2	E	370	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	75	GLN
1	A	78	ASN
1	A	151	HIS
1	A	160	GLN
1	A	195	ASN

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Mol	Chain	Res	Type
1	A	196	ASN
1	A	232	HIS
1	A	267	ASN
1	A	324	ASN
1	A	347	GLN
1	A	368	ASN
2	B	40	HIS
2	B	73	HIS
2	B	88	HIS
2	B	128	ASN
2	B	161	HIS
2	B	246	GLN
2	B	263	GLN
2	B	280	ASN
2	B	353	GLN
1	D	29	HIS
1	D	113	ASN
1	D	151	HIS
1	D	215	GLN
1	D	232	HIS
1	D	267	ASN
1	D	349	GLN
2	E	12	ASN
2	E	73	HIS
2	E	88	HIS
2	E	121	GLN
2	E	225	ASN

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

Of 12 ligands modelled in this entry, 10 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	E	380	3	32,33,33	1.37	4 (12%)	48,52,52	1.83	10 (20%)
4	ATP	B	380	3	32,33,33	1.51	6 (18%)	48,52,52	1.77	10 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	E	380	3	-	1/22/38/38	0/3/3/3
4	ATP	B	380	3	-	3/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	380	ATP	C5-C4	4.80	1.47	1.39
4	E	380	ATP	C5-C4	4.69	1.47	1.39
4	B	380	ATP	PA-O3A	3.05	1.62	1.59
4	B	380	ATP	C5-C6	2.95	1.49	1.41
4	B	380	ATP	C8-N7	2.65	1.36	1.31
4	E	380	ATP	C5-C6	2.65	1.48	1.41
4	E	380	ATP	C8-N7	2.58	1.36	1.31
4	B	380	ATP	PB-O3A	2.37	1.62	1.59
4	B	380	ATP	C4-N9	-2.15	1.33	1.37
4	E	380	ATP	C5-N7	-2.12	1.35	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	380	ATP	C5-C4-N3	-6.03	118.41	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	380	ATP	C5-C4-N3	-4.99	119.84	126.72
4	E	380	ATP	N3-C4-N9	4.59	134.97	127.17
4	B	380	ATP	N3-C4-N9	3.98	133.93	127.17
4	E	380	ATP	C2-N3-C4	3.75	120.99	111.83
4	B	380	ATP	C2-N3-C4	3.61	120.65	111.83
4	B	380	ATP	C4-C5-N7	-3.50	106.58	110.58
4	B	380	ATP	N3-C2-N1	-3.50	123.28	128.58
4	B	380	ATP	C4-N9-C8	3.40	109.31	105.74
4	E	380	ATP	C4-C5-N7	-3.40	106.69	110.58
4	E	380	ATP	O4'-C1'-N9	3.31	114.44	108.09
4	E	380	ATP	N3-C2-N1	-3.04	123.97	128.58
4	B	380	ATP	C6-C5-N7	2.78	137.46	132.09
4	E	380	ATP	O3B-PB-O1B	-2.55	103.03	110.70
4	B	380	ATP	C5-N7-C8	2.52	107.41	103.45
4	B	380	ATP	N9-C8-N7	-2.44	110.47	113.94
4	E	380	ATP	C5-N7-C8	2.43	107.27	103.45
4	E	380	ATP	C4-N9-C8	2.31	108.16	105.74
4	E	380	ATP	C6-C5-N7	2.25	136.43	132.09
4	B	380	ATP	C2-N1-C6	2.07	122.13	118.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	380	ATP	PB-O3B-PG-O2G
4	B	380	ATP	PB-O3B-PG-O3G
4	E	380	ATP	PB-O3B-PG-O2G
4	B	380	ATP	PG-O3B-PB-O2B

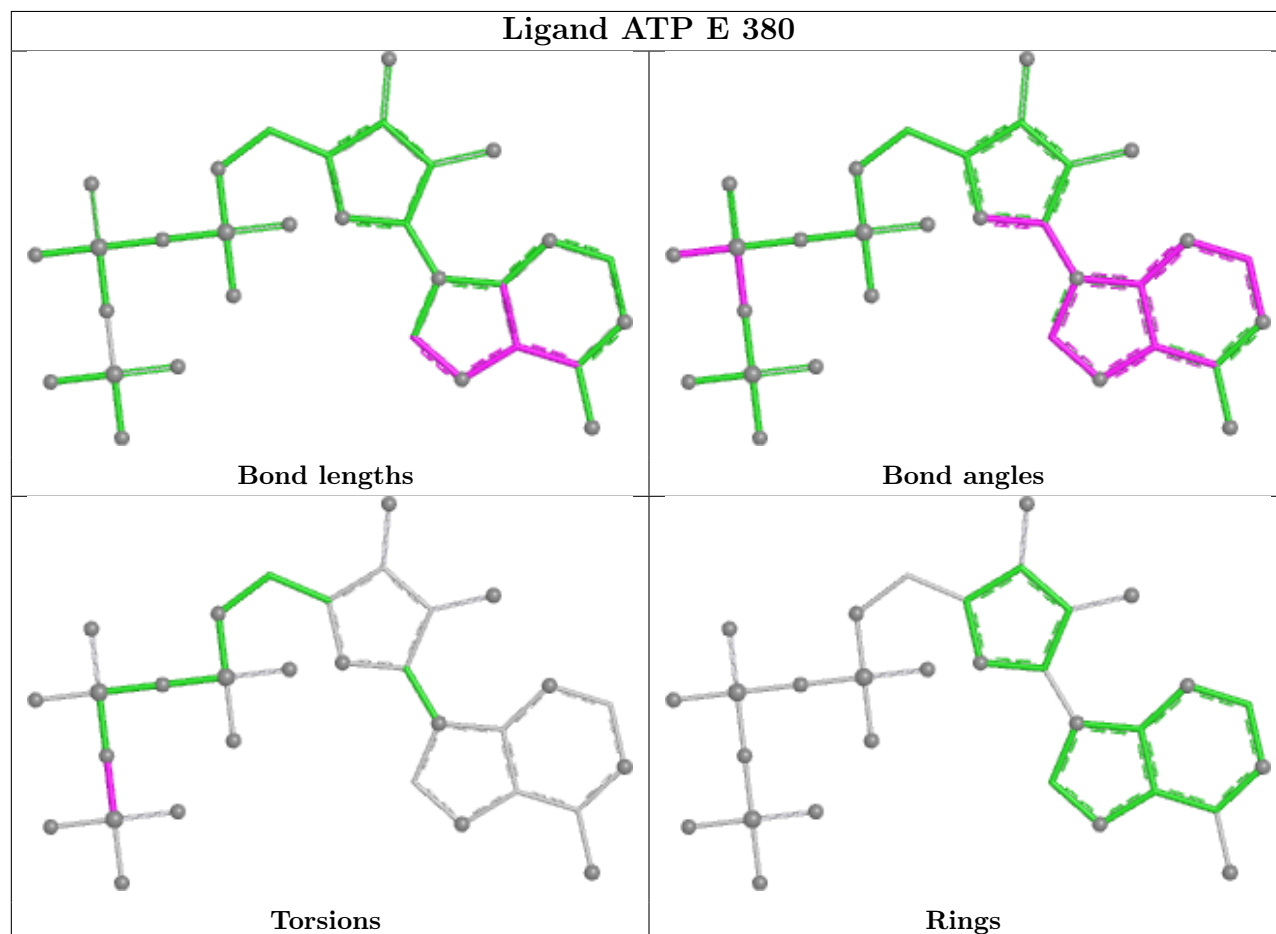
There are no ring outliers.

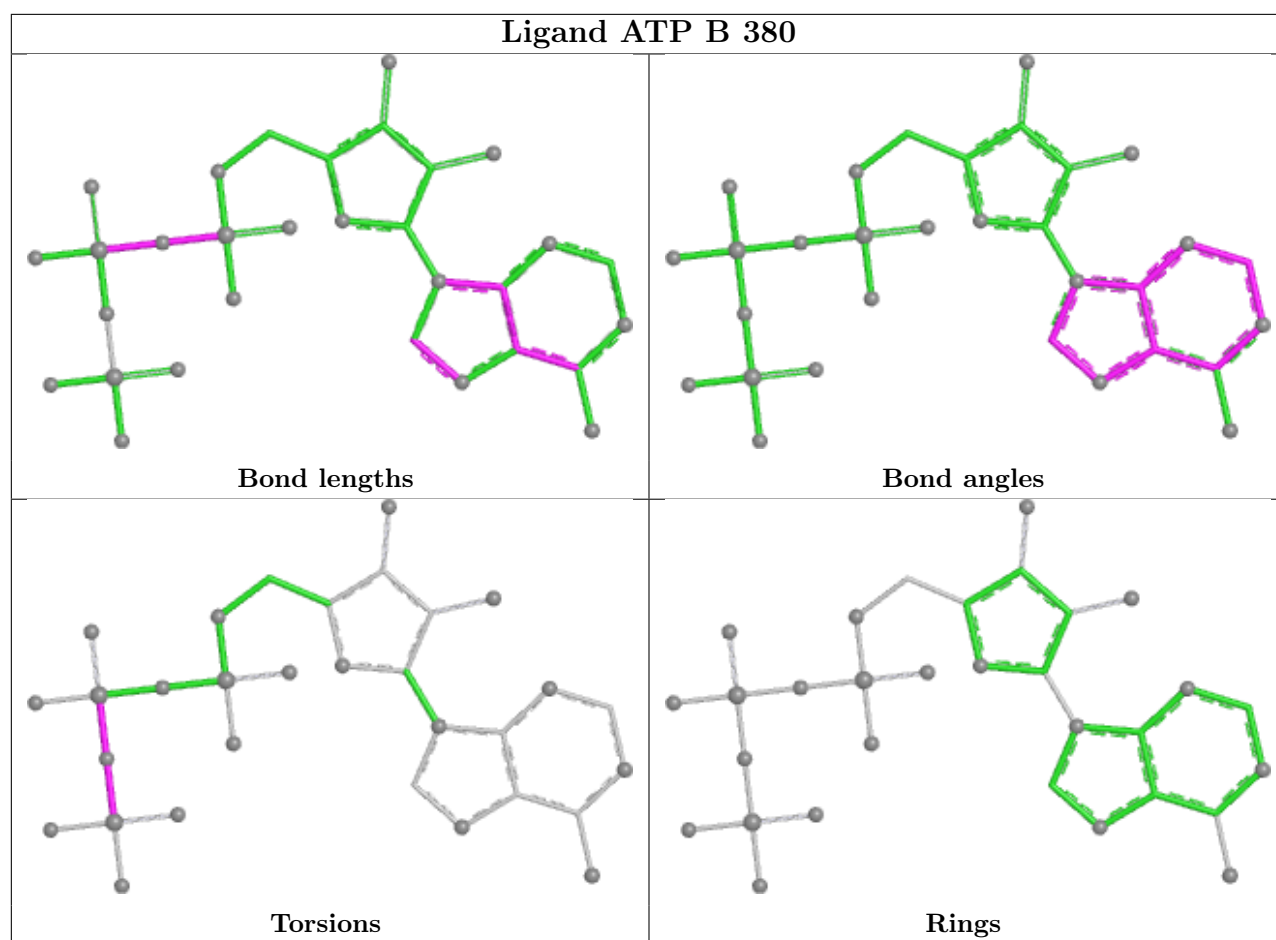
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	380	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 [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, 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	347/377 (92%)	-0.41	1 (0%) 90 79	11, 28, 48, 58	4 (1%)
1	D	346/377 (91%)	-0.34	2 (0%) 85 69	10, 19, 33, 53	1 (0%)
2	B	365/377 (96%)	-0.38	5 (1%) 73 51	7, 16, 33, 57	0
2	E	355/377 (94%)	-0.49	2 (0%) 85 69	8, 17, 30, 37	1 (0%)
All	All	1413/1508 (93%)	-0.40	10 (0%) 84 66	7, 19, 40, 58	6 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	367	PRO	4.1
2	E	370	VAL	3.2
2	B	49	GLN	2.5
2	B	3	ASP	2.5
1	D	27	VAL	2.4
2	B	366	GLY	2.4
1	D	257	THR	2.3
2	E	201	VAL	2.3
2	B	47	MET	2.2
1	A	311[A]	LYS	2.2

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

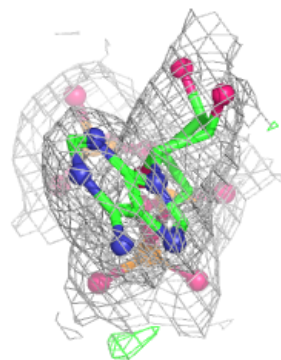
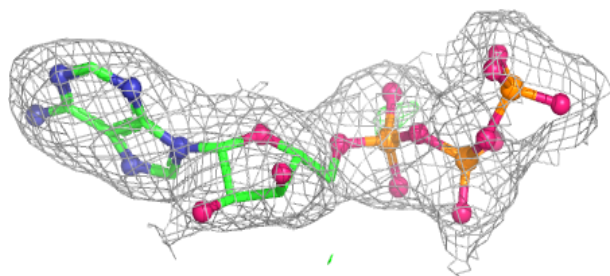
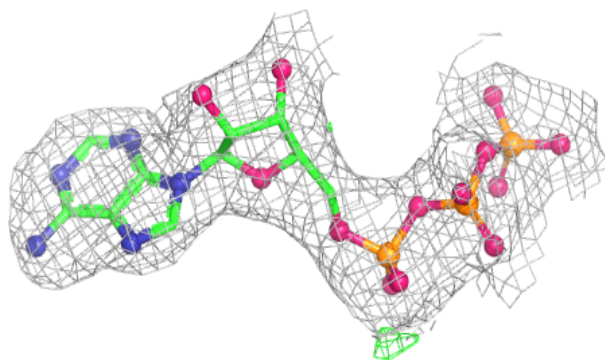
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	A	759	1/1	0.94	0.09	15,15,15,15	0
3	CA	A	758	1/1	0.96	0.04	15,15,15,15	0
3	CA	D	757	1/1	0.98	0.06	28,28,28,28	0
3	CA	D	758	1/1	0.98	0.06	31,31,31,31	0
3	CA	D	759	1/1	0.98	0.06	26,26,26,26	0
4	ATP	E	380	31/31	0.98	0.05	13,18,21,22	0
3	CA	A	757	1/1	0.99	0.07	8,8,8,8	0
3	CA	B	401	1/1	0.99	0.03	7,7,7,7	0
3	CA	E	401	1/1	0.99	0.03	18,18,18,18	0
4	ATP	B	380	31/31	0.99	0.04	7,10,14,14	0
3	CA	A	756	1/1	0.99	0.10	3,3,3,3	0
3	CA	D	756	1/1	1.00	0.01	22,22,22,22	0

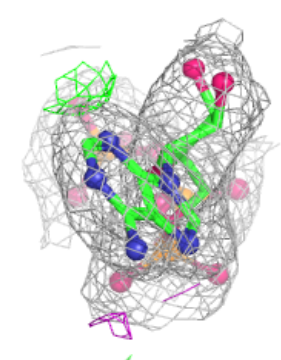
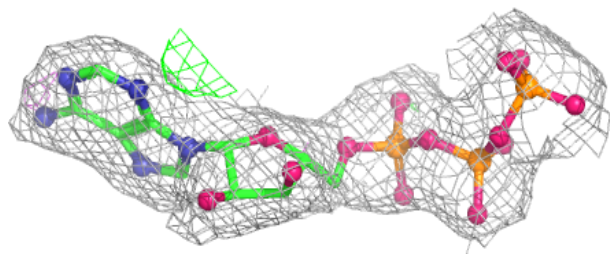
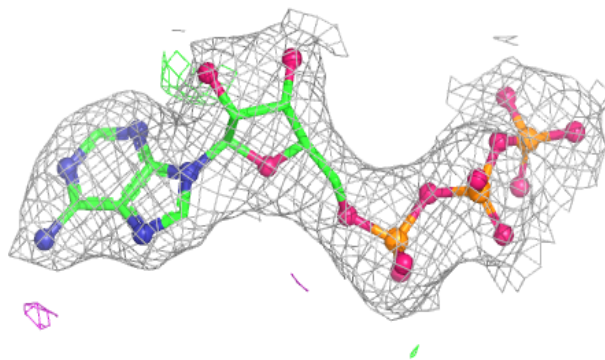
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP E 380:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP B 380:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.