Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 12:38 AM JST

PDB ID	:	7CCC
Title	:	The structure of the actin filament uncapping complex mediated by twinfilin
Authors	:	Robinson, R.C.; Mwangangi, D.M.
Deposited on	:	2020-06-16
Resolution	:	3.20 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 (i)) were used in the production of this report:

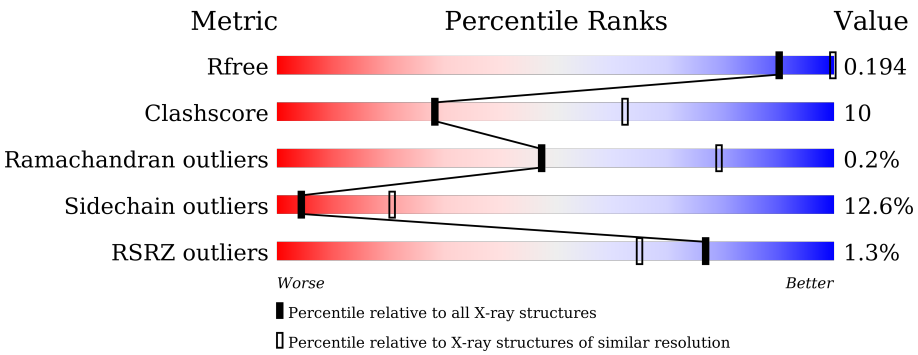
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	A	377	.% 71% 22% • 5%
1	E	377	.% 67% 24% • 5%
2	B	350	67% 26% • •
3	C	286	.% 62% 29% • 6%
4	D	272	2% 58% 30% • 9%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12626 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, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	357	2792	1771	467	536	18	0	0	0
1	E	358	2803	1777	471	537	18	0	0	0

- Molecule 2 is a protein called Twinfilin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	342	2784	1768	487	521	8	0	0	0

- Molecule 3 is a protein called F-actin-capping protein subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	269	2183	1375	379	424	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	222	VAL	ILE	engineered mutation	UNP Q5RKN9

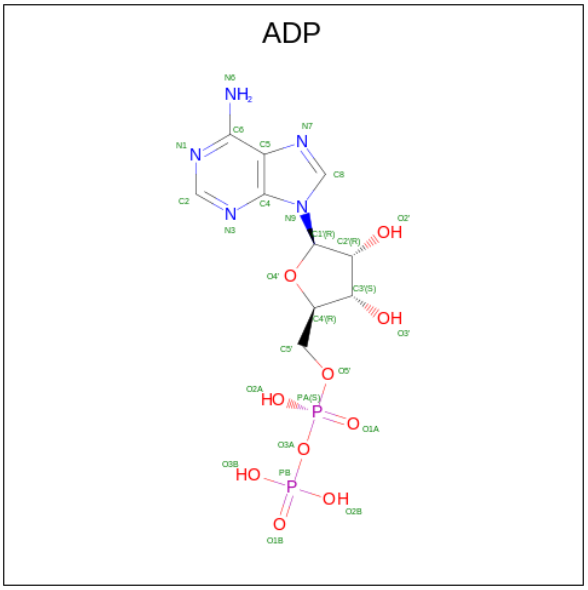
- Molecule 4 is a protein called F-actin-capping protein subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	248	1954	1220	338	385	11	0	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	1	1	1	0	0
5	E	1	1	1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0
6	E	1	27	10	5	10	2	0	0

- Molecule 7 is water.

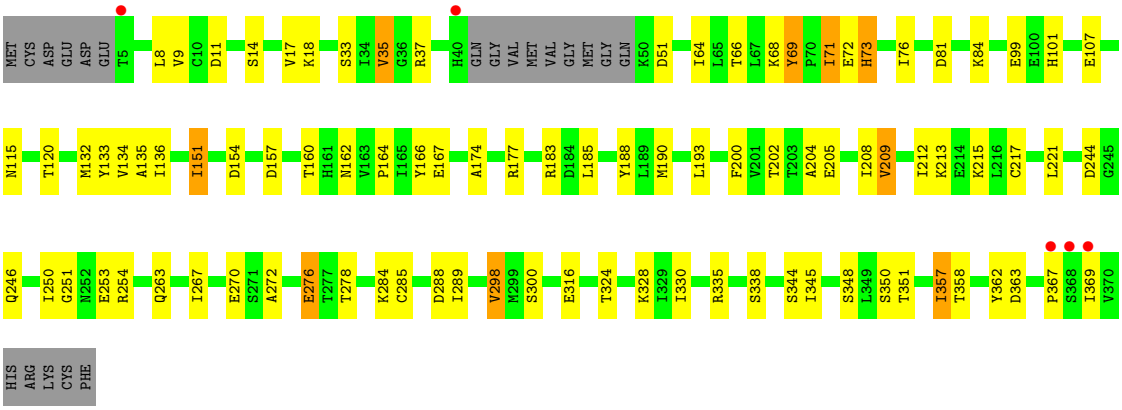
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	20	20	20	0	0
7	B	6	6	6	0	0
7	C	4	4	4	0	0
7	D	1	1	1	0	0
7	E	23	23	23	0	0

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.

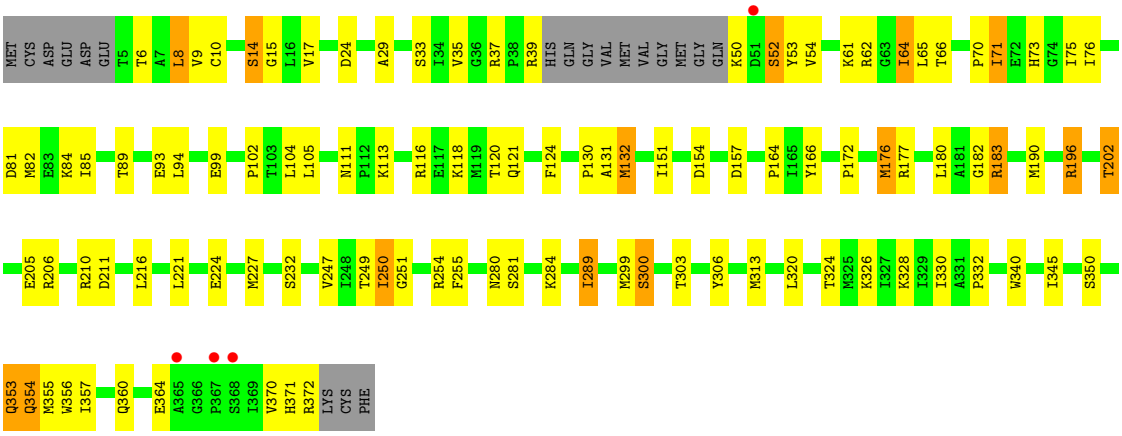
• Molecule 1: Actin, alpha skeletal muscle

Chain A:



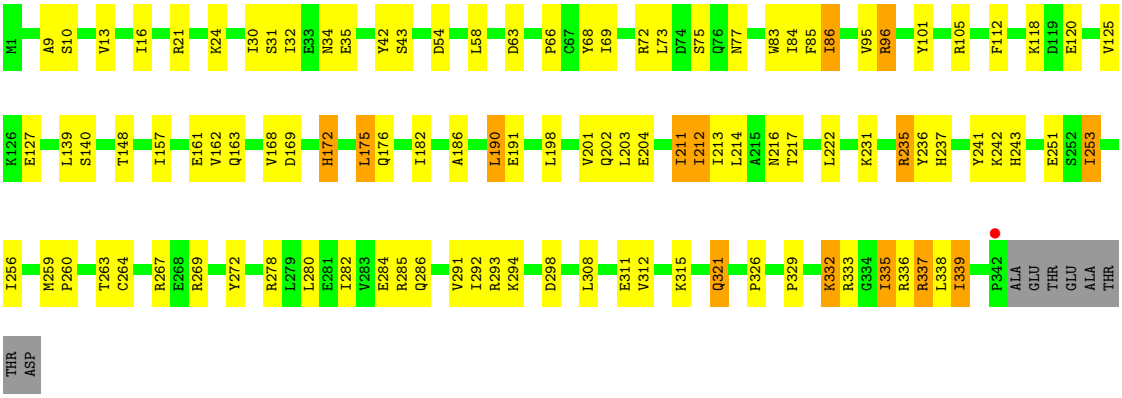
• Molecule 1: Actin, alpha skeletal muscle

Chain E:



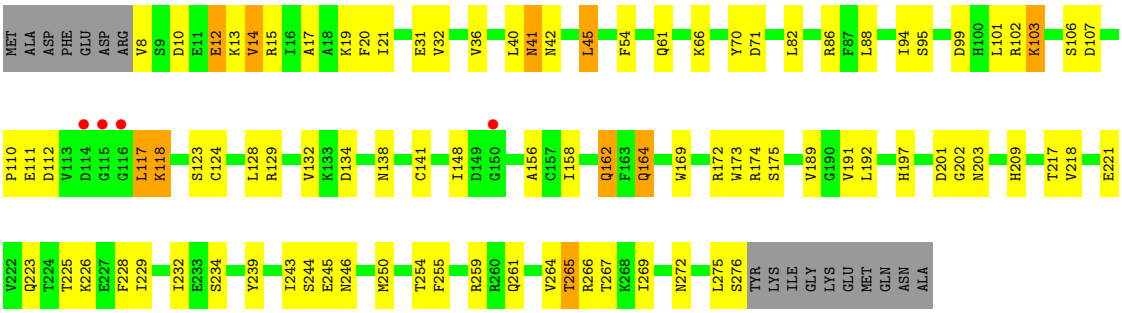
• Molecule 2: Twinfilin-1

Chain B:



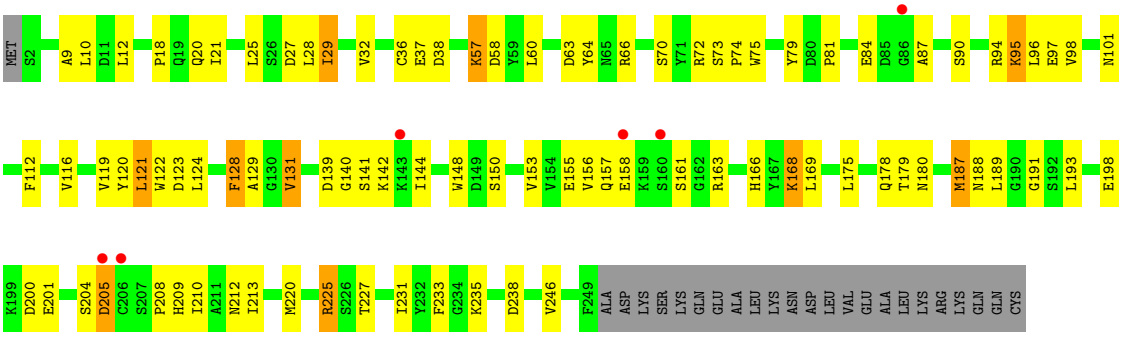
- Molecule 3: F-actin-capping protein subunit alpha

Chain C:



- Molecule 4: F-actin-capping protein subunit beta

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.76Å 168.66Å 176.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 3.20 19.92 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.0 (19.92-3.20) 92.0 (19.92-3.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 3.22Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.186 , 0.238 0.191 , 0.194	Depositor DCC
R_{free} test set	3455 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12626	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: HIC, ADP, 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	0.28	0/2839	0.45	0/3848
1	E	0.28	0/2850	0.48	1/3862 (0.0%)
2	B	0.28	0/2844	0.51	1/3835 (0.0%)
3	C	0.29	0/2233	0.49	1/3028 (0.0%)
4	D	0.29	0/1988	0.50	0/2684
All	All	0.28	0/12754	0.49	3/17257 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	175	LEU	CA-CB-CG	7.54	132.64	115.30
1	E	8	LEU	CA-CB-CG	6.63	130.54	115.30
3	C	117	LEU	CA-CB-CG	6.07	129.25	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2792	0	2763	48	0
1	E	2803	0	2776	59	0
2	B	2784	0	2777	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2183	0	2099	54	0
4	D	1954	0	1931	49	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
6	A	27	0	12	2	0
6	E	27	0	12	1	0
7	A	20	0	0	3	0
7	B	6	0	0	0	0
7	C	4	0	0	2	0
7	D	1	0	0	0	0
7	E	23	0	0	2	0
All	All	12626	0	12370	244	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 10.

All (244) 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)
2:B:326:PRO:HG3	4:D:155:GLU:HB2	1.49	0.92
1:E:196:ARG:NH1	1:E:249:THR:O	2.10	0.85
2:B:202:GLN:HB3	2:B:216:ASN:HB3	1.61	0.82
4:D:97:GLU:HB2	4:D:121:LEU:HD11	1.62	0.81
1:A:69:TYR:HB3	1:A:72:GLU:HB3	1.65	0.77
2:B:332:LYS:NZ	4:D:63:ASP:OD1	2.19	0.76
1:A:35:VAL:HG11	1:A:81:ASP:HB3	1.69	0.75
4:D:148:TRP:NE1	4:D:150:SER:OG	2.20	0.75
4:D:9:ALA:HB1	4:D:28:LEU:HD21	1.68	0.74
1:A:250:ILE:HD11	1:A:253:GLU:HB2	1.70	0.73
1:A:73:HIC:O	1:A:177:ARG:NH2	2.22	0.73
3:C:86:ARG:NH2	3:C:95:SER:OG	2.21	0.73
3:C:265:THR:HB	3:C:267:THR:HG22	1.69	0.73
4:D:79:TYR:OH	4:D:87:ALA:O	2.07	0.73
1:A:244:ASP:HB3	1:A:246:GLN:HG3	1.72	0.72
1:E:166:TYR:HB2	1:E:289:ILE:HD11	1.74	0.70
1:A:284:LYS:NZ	4:D:238:ASP:OD1	2.25	0.70
1:E:76:ILE:HD13	1:E:82:MET:HG2	1.74	0.70
3:C:259:ARG:O	4:D:225:ARG:NH2	2.26	0.69
4:D:18:PRO:HG2	4:D:191:GLY:HA2	1.72	0.69
2:B:264:CYS:O	2:B:269:ARG:NH1	2.26	0.68
1:E:116:ARG:O	1:E:120:THR:HG23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:ARG:HD2	4:D:37:GLU:HG3	1.75	0.67
1:E:157:ASP:OD2	1:E:183:ARG:NH1	2.27	0.67
2:B:337:ARG:HE	4:D:66:ARG:HH11	1.42	0.65
1:A:35:VAL:HG13	1:A:68:LYS:HB2	1.78	0.65
1:E:120:THR:HG21	1:E:370:VAL:HB	1.79	0.65
2:B:96:ARG:HA	1:E:345:ILE:HD13	1.79	0.64
1:E:154:ASP:OD2	7:E:501:HOH:O	2.15	0.64
1:A:188:TYR:HB2	1:A:267:ILE:HD12	1.80	0.64
4:D:25:LEU:O	4:D:29:ILE:HG22	1.98	0.63
1:E:176:MET:HG3	1:E:281:SER:HB2	1.81	0.63
1:A:162:ASN:HD21	1:A:278:THR:HG22	1.64	0.63
2:B:280:LEU:HD13	2:B:294:LYS:HD3	1.80	0.62
3:C:239:TYR:CZ	3:C:243:ILE:HD11	2.34	0.62
1:E:10:CYS:HB3	1:E:105:LEU:HD23	1.81	0.62
4:D:205:ASP:OD1	4:D:205:ASP:N	2.32	0.62
1:A:9:VAL:HG21	1:A:344:SER:HA	1.81	0.61
1:E:353:GLN:HA	1:E:356:TRP:CD1	2.35	0.61
4:D:168:LYS:HE2	4:D:198:GLU:HB2	1.82	0.61
1:E:17:VAL:HG23	1:E:33:SER:HB3	1.82	0.61
2:B:335:ILE:O	4:D:66:ARG:NH1	2.27	0.61
3:C:138:ASN:HD22	3:C:162:GLN:HE21	1.45	0.61
4:D:57:LYS:HB2	4:D:75:TRP:CZ3	2.36	0.60
1:E:53:TYR:HD2	1:E:65:LEU:HD11	1.66	0.60
2:B:293:ARG:NH2	2:B:311:GLU:OE1	2.35	0.60
3:C:41:ASN:O	3:C:41:ASN:ND2	2.35	0.59
1:E:53:TYR:CD2	1:E:65:LEU:HD11	2.37	0.59
1:A:162:ASN:ND2	1:A:278:THR:HG22	2.18	0.58
1:E:29:ALA:HB1	1:E:93:GLU:HG3	1.85	0.58
2:B:253:ILE:HD11	2:B:291:VAL:HG22	1.85	0.57
1:A:208:ILE:O	1:A:212:ILE:HG13	2.04	0.57
1:A:37:ARG:HH21	1:A:84:LYS:HE3	1.68	0.57
2:B:203:LEU:HB2	2:B:236:TYR:HB2	1.87	0.57
1:A:348:SER:OG	2:B:267:ARG:NH2	2.38	0.57
3:C:276:SER:OG	1:E:372:ARG:HB3	2.04	0.56
4:D:29:ILE:HG13	4:D:36:CYS:HB2	1.85	0.56
4:D:166:HIS:HA	4:D:200:ASP:HB3	1.86	0.56
1:E:353:GLN:HA	1:E:356:TRP:HD1	1.70	0.56
1:A:157:ASP:OD1	6:A:402:ADP:O3'	2.21	0.56
1:A:190:MET:HG3	1:A:209:VAL:HG11	1.86	0.56
3:C:40:LEU:HD23	3:C:45:LEU:HD23	1.88	0.55
3:C:128:LEU:HD11	3:C:158:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:GLU:OE1	2:B:235:ARG:NH2	2.39	0.55
4:D:156:VAL:HG21	4:D:213:ILE:HD11	1.89	0.55
4:D:161:SER:HB2	4:D:163:ARG:HG2	1.87	0.55
1:E:154:ASP:OD1	7:E:502:HOH:O	2.18	0.55
1:E:216:LEU:O	1:E:254:ARG:HD2	2.07	0.55
4:D:131:VAL:HG23	4:D:153:VAL:HG22	1.89	0.55
3:C:250:MET:HG2	3:C:254:THR:HB	1.89	0.55
1:E:24:ASP:HB2	1:E:340:TRP:HH2	1.71	0.54
4:D:158:GLU:CD	4:D:209:HIS:HE2	2.10	0.54
1:A:270:GLU:HG2	3:C:261:GLN:HB3	1.89	0.54
3:C:164:GLN:HG3	3:C:169:TRP:CZ2	2.42	0.54
3:C:94:ILE:HG22	3:C:110:PRO:HA	1.90	0.54
3:C:66:LYS:HE3	3:C:70:TYR:O	2.08	0.53
2:B:105:ARG:NH2	2:B:120:GLU:OE2	2.35	0.53
4:D:74:PRO:HG3	4:D:120:TYR:CE2	2.44	0.53
1:E:50:LYS:HD2	1:E:52:SER:O	2.08	0.53
1:A:11:ASP:OD2	7:A:501:HOH:O	2.18	0.53
4:D:140:GLY:HA3	4:D:144:ILE:HB	1.90	0.53
4:D:178:GLN:NE2	4:D:188:ASN:OD1	2.42	0.53
2:B:69:ILE:HB	2:B:86:ILE:HG12	1.90	0.52
1:A:345:ILE:HD13	2:B:267:ARG:HA	1.90	0.52
3:C:21:ILE:HD12	3:C:54:PHE:HE1	1.75	0.52
2:B:292:ILE:HD12	2:B:312:VAL:HG13	1.92	0.52
4:D:58:ASP:N	4:D:75:TRP:HZ3	2.07	0.52
1:A:151:ILE:HD12	1:A:164:PRO:HG3	1.91	0.52
2:B:86:ILE:HG13	2:B:86:ILE:O	2.10	0.52
1:E:9:VAL:HG12	1:E:104:LEU:HB3	1.90	0.51
3:C:17:ALA:O	3:C:21:ILE:HG13	2.10	0.51
2:B:278:ARG:O	2:B:282:ILE:HG12	2.10	0.51
2:B:329:PRO:HD3	4:D:64:TYR:HD2	1.74	0.51
2:B:260:PRO:HD2	2:B:264:CYS:SG	2.50	0.51
1:A:154:ASP:OD1	7:A:502:HOH:O	2.19	0.51
3:C:82:LEU:HD11	3:C:88:LEU:HB2	1.93	0.51
2:B:237:HIS:HB2	2:B:256:ILE:HB	1.92	0.51
2:B:21:ARG:NH1	2:B:112:PHE:O	2.44	0.50
4:D:200:ASP:N	4:D:200:ASP:OD1	2.43	0.50
1:A:200:PHE:HD1	1:A:205:GLU:HB3	1.77	0.50
4:D:95:LYS:HG2	4:D:96:LEU:N	2.27	0.50
1:E:61:LYS:HB3	1:E:64:ILE:HD11	1.93	0.50
1:A:272:ALA:HB1	1:A:276:GLU:HB3	1.92	0.50
2:B:337:ARG:HH11	4:D:66:ARG:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.93	0.49
4:D:70:SER:OG	4:D:81:PRO:O	2.17	0.49
2:B:190:LEU:HD13	2:B:201:VAL:HG11	1.95	0.49
3:C:265:THR:HG22	1:E:172:PRO:HD2	1.94	0.49
3:C:174:ARG:NH2	7:C:301:HOH:O	2.35	0.49
4:D:227:THR:HG23	4:D:231:ILE:HD12	1.95	0.49
1:A:362:TYR:CE1	1:A:367:PRO:HA	2.48	0.48
1:A:166:TYR:CD1	1:A:167:GLU:HG3	2.48	0.48
3:C:12:GLU:HA	3:C:15:ARG:HG2	1.96	0.48
3:C:32:VAL:O	3:C:36:VAL:HG13	2.13	0.48
3:C:61:GLN:HB3	3:C:172:ARG:NH1	2.28	0.48
1:A:166:TYR:CE1	1:A:167:GLU:HG3	2.48	0.48
2:B:32:ILE:HG13	2:B:101:TYR:CE2	2.49	0.48
3:C:10:ASP:O	3:C:14:VAL:HG22	2.14	0.48
1:E:190:MET:HE1	1:E:206:ARG:HA	1.96	0.48
1:A:213:LYS:HA	1:A:217:CYS:SG	2.54	0.47
1:E:35:VAL:HG22	1:E:54:VAL:HG22	1.95	0.47
2:B:339:ILE:H	2:B:339:ILE:HG12	1.40	0.47
3:C:259:ARG:HG3	4:D:112:PHE:CE2	2.49	0.47
4:D:128:PHE:N	4:D:128:PHE:CD2	2.82	0.47
3:C:31:GLU:OE1	3:C:31:GLU:N	2.47	0.47
1:E:151:ILE:HD12	1:E:164:PRO:HG3	1.95	0.47
3:C:99:ASP:O	3:C:103:LYS:HA	2.14	0.47
3:C:164:GLN:HG3	3:C:169:TRP:CH2	2.49	0.47
3:C:138:ASN:ND2	3:C:162:GLN:HE21	2.12	0.47
4:D:178:GLN:HA	4:D:187:MET:O	2.15	0.47
4:D:210:ILE:HD12	4:D:210:ILE:H	1.80	0.47
1:A:17:VAL:HG23	1:A:33:SER:HB3	1.97	0.47
1:A:18:LYS:NZ	6:A:402:ADP:O1A	2.43	0.47
1:E:70:PRO:HG2	1:E:85:ILE:HD12	1.97	0.47
2:B:125:VAL:HG23	2:B:127:GLU:H	1.80	0.46
4:D:208:PRO:O	4:D:212:ASN:ND2	2.48	0.46
1:A:133:TYR:HE2	1:A:135:ALA:HB2	1.81	0.46
1:E:166:TYR:CB	1:E:289:ILE:HD11	2.42	0.46
4:D:18:PRO:O	4:D:21:ILE:HG13	2.15	0.46
3:C:103:LYS:HE2	3:C:103:LYS:HB2	1.53	0.46
3:C:192:LEU:O	3:C:209:HIS:HA	2.16	0.46
1:E:227:MET:HG2	1:E:255:PHE:HE1	1.80	0.46
2:B:337:ARG:CZ	2:B:337:ARG:HB2	2.45	0.46
1:E:306:TYR:CE1	6:E:402:ADP:H2	2.33	0.46
2:B:9:ALA:HB1	2:B:13:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LEU:HD21	2:B:84:ILE:HD11	1.98	0.46
2:B:285:ARG:HH21	2:B:286:GLN:HG3	1.80	0.46
3:C:42:ASN:HB3	3:C:45:LEU:HB3	1.97	0.45
2:B:72:ARG:HG3	2:B:83:TRP:CZ2	2.51	0.45
2:B:211:ILE:HG12	2:B:212:ILE:N	2.32	0.45
1:E:166:TYR:CG	1:E:289:ILE:HD11	2.51	0.45
1:A:270:GLU:OE2	3:C:266:ARG:NE	2.49	0.45
1:E:102:PRO:HB3	1:E:131:ALA:HB3	1.98	0.45
1:A:357:ILE:HG21	1:A:369:ILE:HG12	1.98	0.45
3:C:229:ILE:HD13	3:C:229:ILE:HA	1.80	0.45
1:A:204:ALA:O	1:A:208:ILE:HG12	2.17	0.45
3:C:228:PHE:CZ	3:C:232:ILE:HD11	2.51	0.45
1:E:116:ARG:HG2	1:E:370:VAL:HG21	1.97	0.45
3:C:173:TRP:HE1	3:C:175:SER:HB2	1.82	0.45
1:E:330:ILE:HG22	1:E:332:PRO:HD3	1.99	0.45
3:C:229:ILE:HD13	3:C:232:ILE:HD12	1.99	0.45
1:E:182:GLY:CA	1:E:303:THR:HG21	2.47	0.45
1:E:89:THR:O	1:E:94:LEU:HB2	2.17	0.45
3:C:124:CYS:SG	3:C:225:THR:HG22	2.57	0.44
1:A:8:LEU:HD13	1:A:101:HIS:HB3	1.99	0.44
1:A:193:LEU:HD21	1:A:250:ILE:HD13	2.00	0.44
2:B:30:ILE:HB	2:B:68:TYR:HB2	1.98	0.44
2:B:34:ASN:O	2:B:35:GLU:HG2	2.18	0.44
3:C:197:HIS:NE2	3:C:203:ASN:OD1	2.40	0.44
3:C:221:GLU:OE1	3:C:221:GLU:N	2.43	0.44
1:E:300:SER:O	1:E:300:SER:OG	2.33	0.44
3:C:86:ARG:NH1	3:C:107:ASP:OD1	2.49	0.44
3:C:118:LYS:HE2	3:C:118:LYS:HB2	1.68	0.44
2:B:85:PHE:HD2	2:B:120:GLU:HG3	1.83	0.44
1:E:99:GLU:O	1:E:130:PRO:HG3	2.18	0.44
1:E:118:LYS:O	1:E:121:GLN:HB2	2.18	0.44
2:B:222:LEU:HD11	2:B:308:LEU:HD12	2.00	0.44
1:A:164:PRO:HG2	1:A:174:ALA:CB	2.48	0.43
2:B:216:ASN:OD1	2:B:217:THR:N	2.51	0.43
3:C:202:GLY:HA3	4:D:193:LEU:HD23	1.99	0.43
1:E:113:LYS:HB3	1:E:371:HIS:CE1	2.53	0.43
1:A:154:ASP:O	1:A:160:THR:HA	2.18	0.43
2:B:68:TYR:CE2	2:B:105:ARG:HG3	2.54	0.43
3:C:21:ILE:HD11	3:C:36:VAL:HG21	2.00	0.43
3:C:132:VAL:HG21	3:C:141:CYS:HB3	2.00	0.43
4:D:72:ARG:HA	4:D:79:TYR:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HA	1:A:338:SER:HB3	1.99	0.43
1:A:190:MET:HG2	1:A:200:PHE:HB3	2.00	0.43
4:D:60:LEU:HD23	4:D:60:LEU:HA	1.77	0.43
1:E:216:LEU:HD22	1:E:250:ILE:HD11	2.01	0.43
4:D:94:ARG:O	4:D:98:VAL:HG23	2.18	0.43
4:D:122:TRP:CE2	4:D:129:ALA:HB3	2.54	0.43
1:E:124:PHE:CZ	1:E:132:MET:HG2	2.54	0.43
1:A:157:ASP:OD2	1:A:183:ARG:HD3	2.19	0.43
2:B:66:PRO:HB2	2:B:101:TYR:CD1	2.53	0.43
1:E:350:SER:O	1:E:353:GLN:HB3	2.18	0.43
2:B:241:TYR:CE1	2:B:243:HIS:HB3	2.53	0.42
3:C:13:LYS:HB3	3:C:13:LYS:HE3	1.66	0.42
3:C:172:ARG:HB3	7:C:301:HOH:O	2.20	0.42
1:E:120:THR:HG21	1:E:370:VAL:CB	2.48	0.42
1:E:328:LYS:HD3	1:E:330:ILE:HD11	2.01	0.42
2:B:236:TYR:OH	2:B:272:TYR:O	2.31	0.42
3:C:123:SER:HB3	3:C:225:THR:HG21	2.00	0.42
2:B:186:ALA:HA	2:B:214:LEU:HB2	2.01	0.42
1:A:120:THR:HG23	1:A:132:MET:SD	2.59	0.42
2:B:242:LYS:HG2	2:B:251:GLU:HG2	2.02	0.42
4:D:193:LEU:HD23	4:D:193:LEU:HA	1.90	0.42
1:E:111:ASN:O	1:E:116:ARG:NH2	2.52	0.42
2:B:186:ALA:HB1	2:B:203:LEU:HD11	2.00	0.42
1:E:299:MET:CE	1:E:313:MET:HG3	2.50	0.42
1:A:71:ILE:HG23	1:A:76:ILE:HG12	2.02	0.42
1:A:136:ILE:HD11	2:B:172:HIS:O	2.18	0.42
1:A:263:GLN:HB3	7:A:509:HOH:O	2.20	0.42
2:B:125:VAL:HG23	2:B:127:GLU:N	2.35	0.42
4:D:29:ILE:O	4:D:29:ILE:HG12	2.20	0.42
4:D:119:VAL:HA	4:D:131:VAL:O	2.20	0.41
3:C:111:GLU:HA	3:C:111:GLU:OE1	2.20	0.41
3:C:269:ILE:HD12	3:C:269:ILE:HA	1.81	0.41
1:E:360:GLN:O	1:E:364:GLU:HG3	2.20	0.41
1:E:61:LYS:HE3	1:E:64:ILE:HD11	2.03	0.41
1:A:107:GLU:HB2	1:A:134:VAL:HG12	2.03	0.41
1:E:353:GLN:HG2	1:E:354:GLN:N	2.34	0.41
3:C:20:PHE:CD1	4:D:12:LEU:HD21	2.55	0.41
1:E:280:ASN:O	1:E:284:LYS:HG3	2.20	0.41
1:A:251:GLY:O	1:A:254:ARG:HG3	2.20	0.41
2:B:72:ARG:HG3	2:B:83:TRP:CE2	2.56	0.41
1:E:182:GLY:HA3	1:E:303:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:PRO:HA	2:B:298:ASP:O	2.21	0.41
4:D:189:LEU:HD21	4:D:233:PHE:CG	2.55	0.41
1:E:37:ARG:CG	1:E:52:SER:HB3	2.51	0.41
1:E:70:PRO:HG3	1:E:81:ASP:HB3	2.02	0.41
1:E:303:THR:HB	1:E:306:TYR:HE2	1.86	0.41
4:D:128:PHE:N	4:D:128:PHE:HD2	2.18	0.41
1:E:64:ILE:H	1:E:64:ILE:HG12	1.64	0.41
1:E:202:THR:HG23	1:E:205:GLU:CD	2.40	0.40
3:C:54:PHE:CE2	3:C:101:LEU:HD21	2.55	0.40
3:C:128:LEU:O	3:C:132:VAL:HG23	2.21	0.40
2:B:280:LEU:O	2:B:284:GLU:HG3	2.21	0.40
3:C:99:ASP:CG	3:C:102:ARG:HE	2.25	0.40
3:C:128:LEU:HD22	3:C:156:ALA:HB1	2.04	0.40
2:B:157:ILE:O	2:B:161:GLU:HB2	2.22	0.40
1:A:298:VAL:HA	1:A:330:ILE:O	2.22	0.40
2:B:321:GLN:H	2:B:321:GLN:HG3	1.64	0.40
1:E:14:SER:HA	1:E:71:ILE:O	2.22	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	352/377 (93%)	343 (97%)	9 (3%)	0	100	100
1	E	353/377 (94%)	341 (97%)	10 (3%)	2 (1%)	25	64
2	B	340/350 (97%)	326 (96%)	14 (4%)	0	100	100
3	C	267/286 (93%)	257 (96%)	10 (4%)	0	100	100
4	D	246/272 (90%)	234 (95%)	11 (4%)	1 (0%)	34	69
All	All	1558/1662 (94%)	1501 (96%)	54 (4%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	141	SER
1	E	251	GLY
1	E	15	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	302/319 (95%)	275 (91%)	27 (9%)	9	35
1	E	303/319 (95%)	269 (89%)	34 (11%)	6	25
2	B	304/310 (98%)	259 (85%)	45 (15%)	3	14
3	C	241/255 (94%)	208 (86%)	33 (14%)	3	17
4	D	220/241 (91%)	186 (84%)	34 (16%)	2	12
All	All	1370/1444 (95%)	1197 (87%)	173 (13%)	4	21

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	35	VAL
1	A	51	ASP
1	A	64	ILE
1	A	66	THR
1	A	69	TYR
1	A	71	ILE
1	A	99	GLU
1	A	115	ASN
1	A	151	ILE
1	A	185	LEU
1	A	202	THR
1	A	209	VAL
1	A	215	LYS
1	A	221	LEU

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Mol	Chain	Res	Type
1	A	276	GLU
1	A	288	ASP
1	A	298	VAL
1	A	300	SER
1	A	316	GLU
1	A	324	THR
1	A	328	LYS
1	A	350	SER
1	A	351	THR
1	A	357	ILE
1	A	358	THR
1	A	363	ASP
2	B	10	SER
2	B	16	ILE
2	B	24	LYS
2	B	31	SER
2	B	42	TYR
2	B	43	SER
2	B	54	ASP
2	B	58	LEU
2	B	63	ASP
2	B	75	SER
2	B	77	ASN
2	B	86	ILE
2	B	95	VAL
2	B	96	ARG
2	B	118	LYS
2	B	139	LEU
2	B	140	SER
2	B	148	THR
2	B	162	VAL
2	B	163	GLN
2	B	168	VAL
2	B	169	ASP
2	B	172	HIS
2	B	175	LEU
2	B	176	GLN
2	B	182	ILE
2	B	190	LEU
2	B	191	GLU
2	B	198	LEU
2	B	211	ILE

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Mol	Chain	Res	Type
2	B	212	ILE
2	B	213	ILE
2	B	231	LYS
2	B	235	ARG
2	B	253	ILE
2	B	259	MET
2	B	263	THR
2	B	315	LYS
2	B	321	GLN
2	B	332	LYS
2	B	333	ARG
2	B	335	ILE
2	B	337	ARG
2	B	338	LEU
2	B	339	ILE
3	C	8	VAL
3	C	12	GLU
3	C	14	VAL
3	C	19	LYS
3	C	41	ASN
3	C	45	LEU
3	C	71	ASP
3	C	103	LYS
3	C	106	SER
3	C	112	ASP
3	C	117	LEU
3	C	118	LYS
3	C	129	ARG
3	C	134	ASP
3	C	148	ILE
3	C	162	GLN
3	C	164	GLN
3	C	189	VAL
3	C	191	VAL
3	C	201	ASP
3	C	217	THR
3	C	218	VAL
3	C	223	GLN
3	C	226	LYS
3	C	234	SER
3	C	244	SER
3	C	245	GLU

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Mol	Chain	Res	Type
3	C	246	ASN
3	C	255	PHE
3	C	264	VAL
3	C	265	THR
3	C	272	ASN
3	C	275	LEU
4	D	10	LEU
4	D	20	GLN
4	D	27	ASP
4	D	29	ILE
4	D	32	VAL
4	D	38	ASP
4	D	57	LYS
4	D	73	SER
4	D	84	GLU
4	D	90	SER
4	D	95	LYS
4	D	101	ASN
4	D	116	VAL
4	D	121	LEU
4	D	123	ASP
4	D	124	LEU
4	D	128	PHE
4	D	131	VAL
4	D	139	ASP
4	D	142	LYS
4	D	157	GLN
4	D	168	LYS
4	D	169	LEU
4	D	175	LEU
4	D	179	THR
4	D	180	ASN
4	D	187	MET
4	D	201	GLU
4	D	204	SER
4	D	205	ASP
4	D	220	MET
4	D	225	ARG
4	D	235	LYS
4	D	246	VAL
1	E	6	THR
1	E	8	LEU

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Mol	Chain	Res	Type
1	E	14	SER
1	E	39	ARG
1	E	52	SER
1	E	62	ARG
1	E	64	ILE
1	E	66	THR
1	E	71	ILE
1	E	75	ILE
1	E	84	LYS
1	E	132	MET
1	E	176	MET
1	E	177	ARG
1	E	180	LEU
1	E	183	ARG
1	E	196	ARG
1	E	202	THR
1	E	210	ARG
1	E	211	ASP
1	E	221	LEU
1	E	224	GLU
1	E	232	SER
1	E	247	VAL
1	E	250	ILE
1	E	289	ILE
1	E	300	SER
1	E	320	LEU
1	E	324	THR
1	E	326	LYS
1	E	353	GLN
1	E	354	GLN
1	E	355	MET
1	E	357	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	243	HIS
3	C	138	ASN
4	D	178	GLN
4	D	188	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HIC	E	73	1	8,11,12	1.74	2 (25%)	6,14,16	1.13	1 (16%)
1	HIC	A	73	1	8,11,12	1.70	2 (25%)	6,14,16	1.10	0

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
1	HIC	E	73	1	-	2/5/6/8	0/1/1/1
1	HIC	A	73	1	-	0/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	73	HIC	CD2-CG	3.77	1.41	1.36
1	A	73	HIC	CD2-CG	3.73	1.41	1.36
1	A	73	HIC	CZ-NE2	-2.22	1.42	1.48
1	E	73	HIC	CZ-NE2	-2.07	1.42	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	73	HIC	CB-CA-C	-2.01	107.71	111.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	73	HIC	CA-CB-CG-ND1
1	E	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	1	0

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ADP	E	402	5	24,29,29	0.93	1 (4%)	29,45,45	1.40	3 (10%)
6	ADP	A	402	5	24,29,29	0.93	1 (4%)	29,45,45	1.35	4 (13%)

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
6	ADP	E	402	5	-	3/12/32/32	0/3/3/3
6	ADP	A	402	5	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	402	ADP	C5-C4	2.39	1.47	1.40
6	A	402	ADP	C5-C4	2.36	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	402	ADP	PA-O3A-PB	-3.70	120.14	132.83
6	A	402	ADP	N3-C2-N1	-3.10	123.83	128.68
6	A	402	ADP	C3'-C2'-C1'	3.07	105.61	100.98
6	E	402	ADP	C4-C5-N7	-2.91	106.37	109.40
6	E	402	ADP	N3-C2-N1	-2.80	124.30	128.68
6	A	402	ADP	PA-O3A-PB	-2.58	123.98	132.83
6	A	402	ADP	C4-C5-N7	-2.57	106.72	109.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	402	ADP	O4'-C4'-C5'-O5'
6	A	402	ADP	C3'-C4'-C5'-O5'
6	E	402	ADP	C3'-C4'-C5'-O5'
6	E	402	ADP	O4'-C4'-C5'-O5'
6	A	402	ADP	C5'-O5'-PA-O1A
6	E	402	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

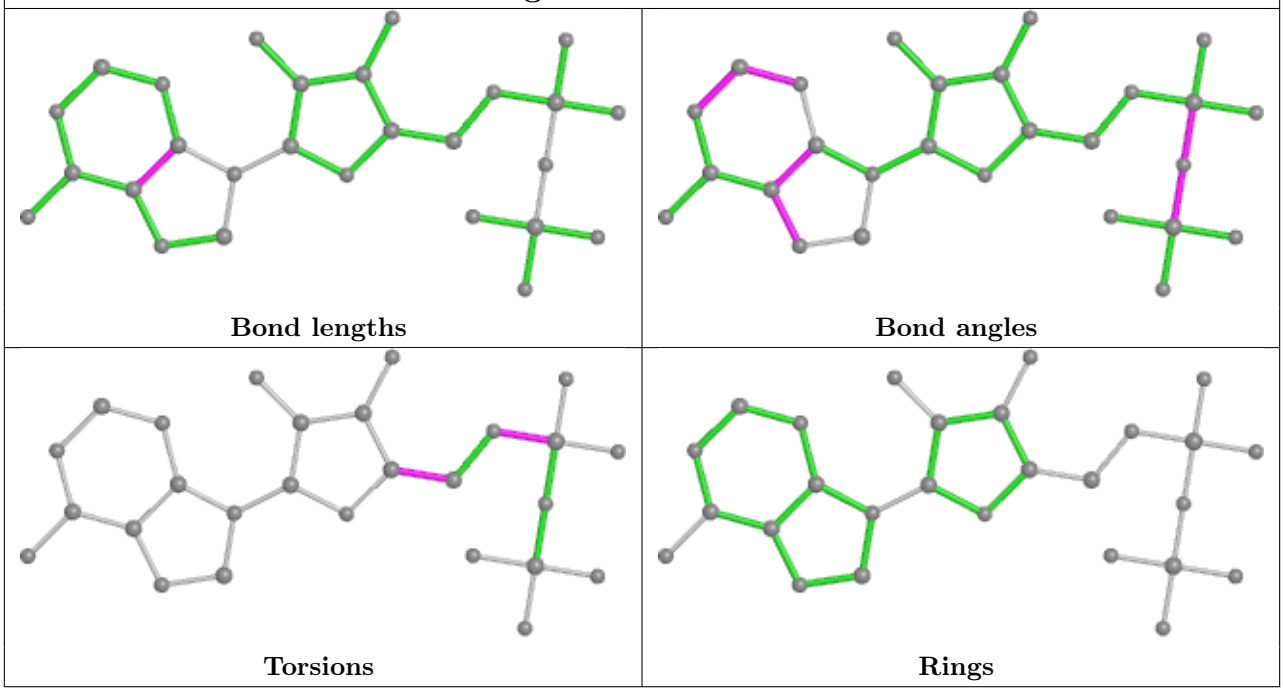
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	402	ADP	1	0
6	A	402	ADP	2	0

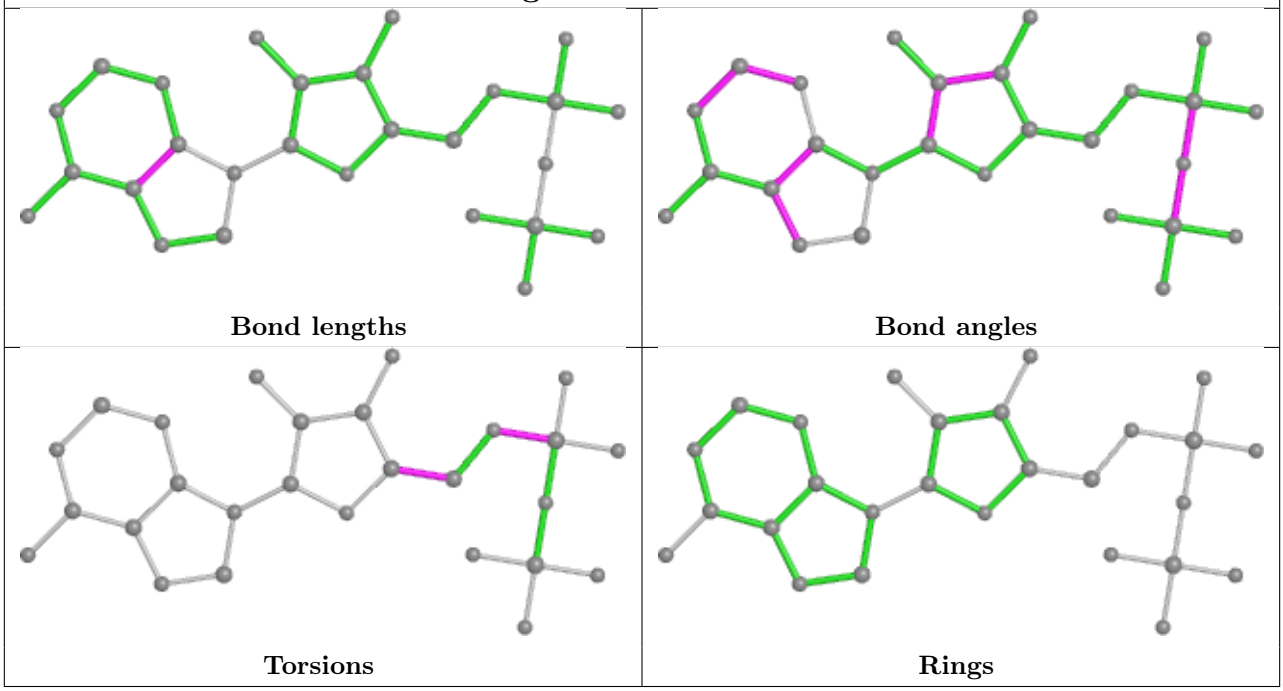
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand ADP E 402



Ligand ADP A 402



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	356/377 (94%)	-0.46	5 (1%)	75	63	18, 47, 102, 137	0
1	E	357/377 (94%)	-0.47	4 (1%)	80	69	19, 46, 97, 150	0
2	B	342/350 (97%)	-0.43	1 (0%)	94	92	20, 51, 103, 142	0
3	C	269/286 (94%)	-0.49	4 (1%)	73	61	20, 48, 87, 127	0
4	D	248/272 (91%)	-0.24	6 (2%)	59	44	22, 68, 116, 138	0
All	All	1572/1662 (94%)	-0.43	20 (1%)	77	65	18, 51, 104, 150	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	SER	6.2
1	A	369	ILE	4.7
4	D	206	CYS	4.0
4	D	205	ASP	4.0
1	E	367	PRO	4.0
1	A	367	PRO	3.3
3	C	114	ASP	2.7
1	A	40	HIS	2.7
2	B	342	PRO	2.6
1	E	368	SER	2.5
3	C	115	GLY	2.5
3	C	116	GLY	2.3
1	E	51	ASP	2.2
4	D	143	LYS	2.2
4	D	158	GLU	2.2
4	D	160	SER	2.1
3	C	150	GLY	2.1
1	E	365	ALA	2.1
1	A	5	THR	2.1
4	D	86	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
1	HIC	A	73	11/12	0.94	0.17	39,49,55,56	0
1	HIC	E	73	11/12	0.94	0.19	56,85,89,95	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

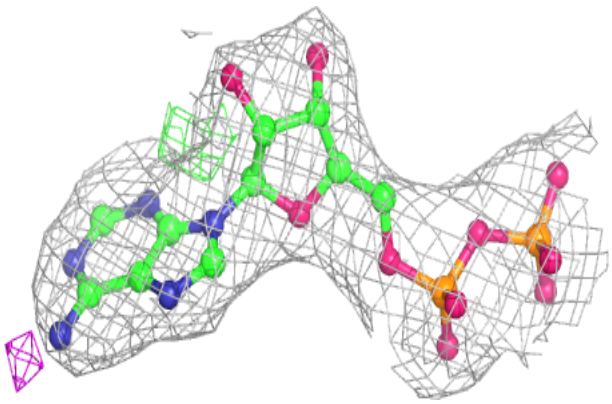
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

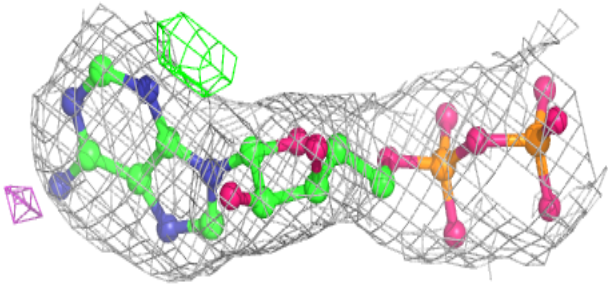
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ADP	E	402	27/27	0.97	0.13	23,25,43,47	0
6	ADP	A	402	27/27	0.98	0.13	23,33,50,66	0
5	CA	A	401	1/1	0.98	0.08	51,51,51,51	0
5	CA	E	401	1/1	1.00	0.11	43,43,43,43	0

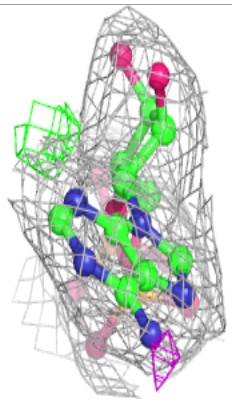
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP E 402:

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

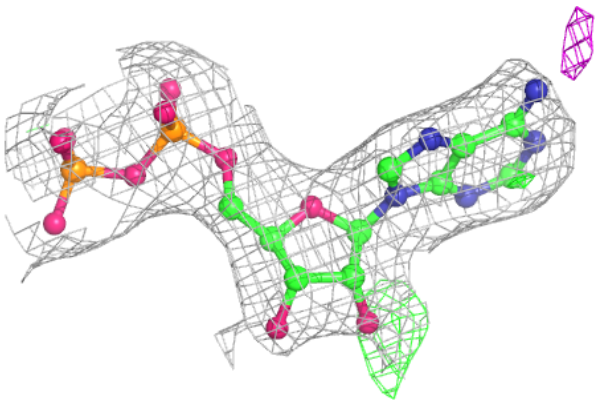


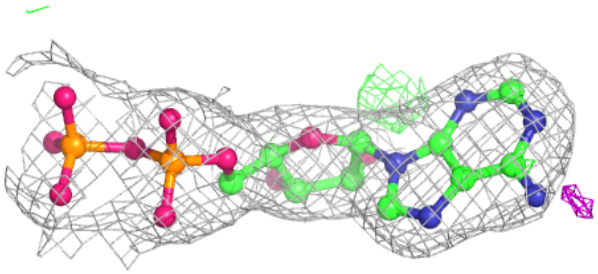


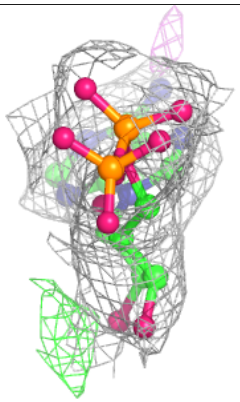


Electron density around ADP A 402:

$2mF_o$-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.