Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 09:08 AM EDT

PDB ID	:	1MDU
Title	:	Crystal structure of the chicken actin trimer complexed with human gelsolin segment 1 (GS-1)
Authors	:	Dawson, J.F.; Sablin, E.P.; Spudich, J.A.; Fletterick, R.J.
Deposited on	:	2002-08-07
Resolution	:	2.20 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:

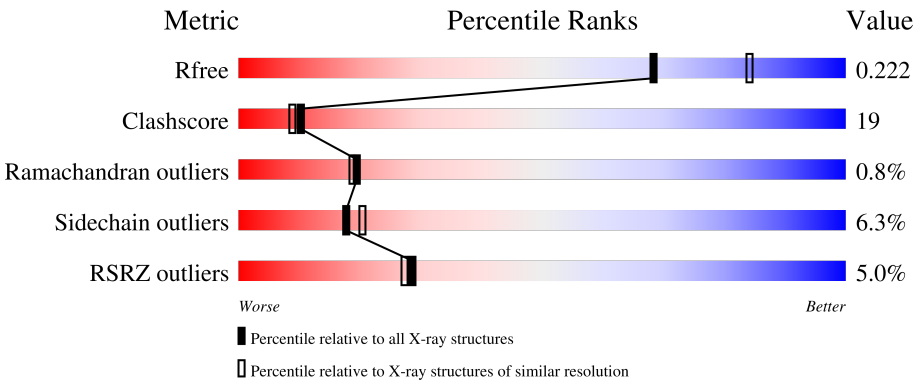
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	125	3% 72% 25%
1	D	125	3% 77% 21%
2	B	377	4% 64% 27%
2	E	377	7% 66% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRS	A	472	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8159 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 gelsolin precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	124	989	640	164	184	1	0	0	0
1	D	123	982	635	163	183	1	0	0	0

- Molecule 2 is a protein called a-actin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	361	2815	1784	472	541	18	0	0	0
2	E	362	2825	1790	475	542	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

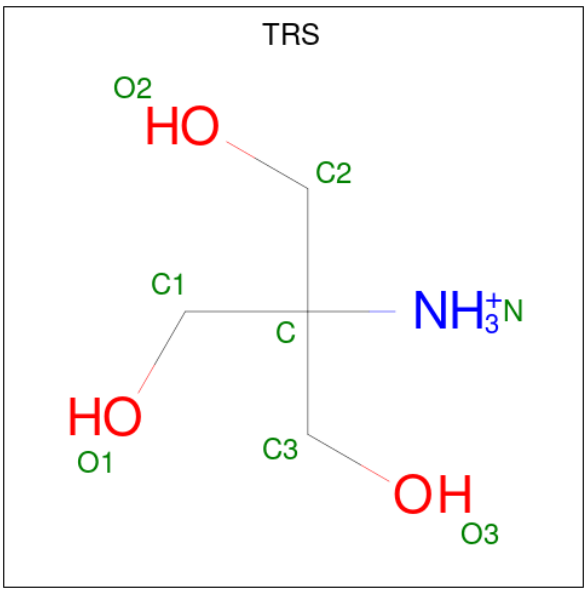
Chain	Residue	Modelled	Actual	Comment	Reference
B	75	HIC	HIS	MODIFIED RESIDUE	UNP P68139
E	75	HIC	HIS	MODIFIED RESIDUE	UNP P68139

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	D	2	2	2	0	0
3	E	1	1	1	0	0

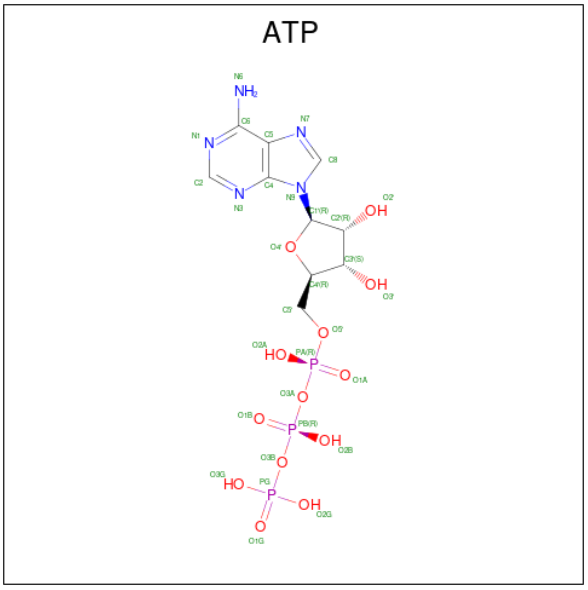
- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code:

TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	8	4	1	3	0	0

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



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

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

- Molecule 6 is water.

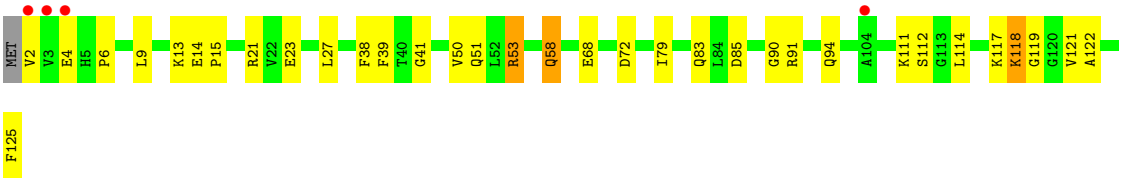
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	67	67	67	0	0
			Total	O		
6	B	179	179	179	0	0
			Total	O		
6	D	64	64	64	0	0
			Total	O		
6	E	161	161	161	0	0

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: gelsolin precursor

Chain A:

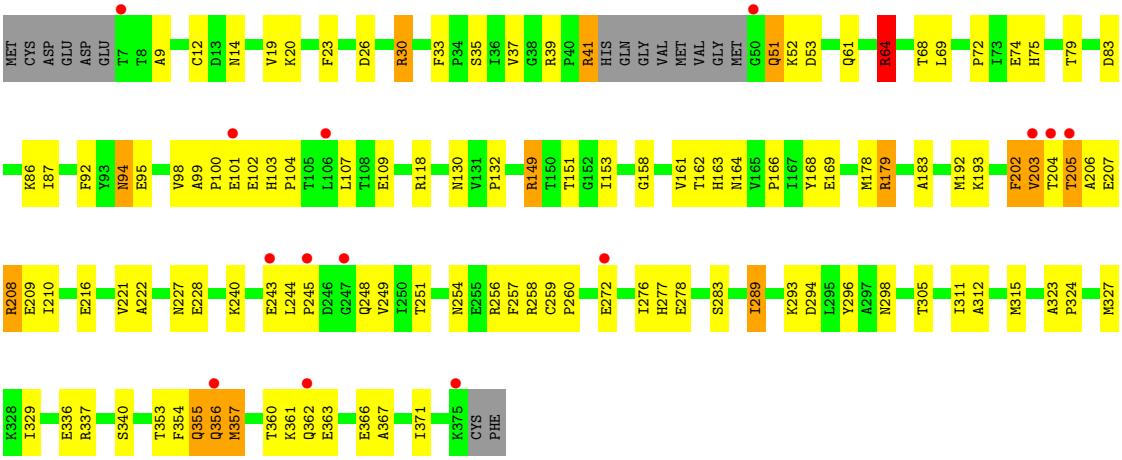


• Molecule 1: gelsolin precursor

Chain D:

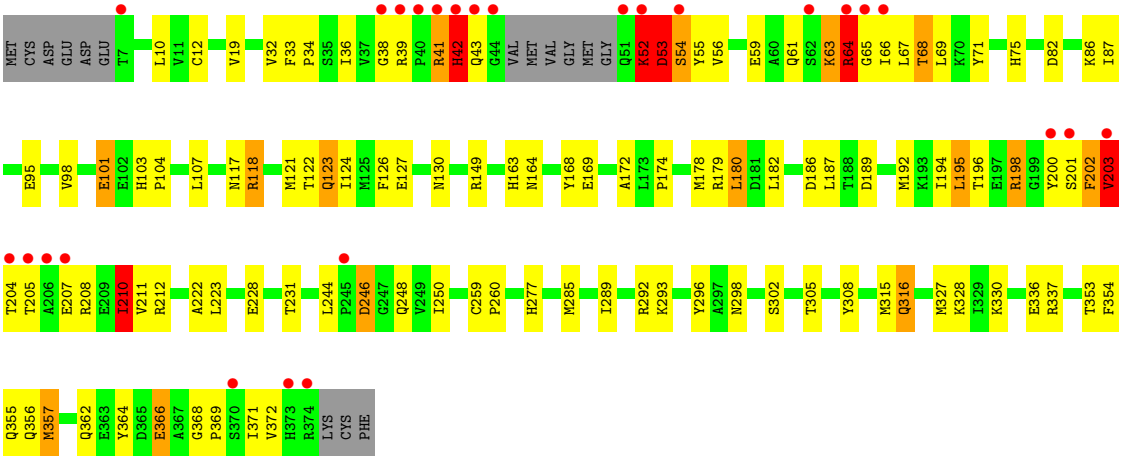
• Molecule 2: a-actin

Chain B:



• Molecule 2: a-actin

Chain E:


MET CYS ASP GLU ASP GLU T7 L10 V11 C12 V19 V32 F33 P34 S35 I36 V37 G38 R39 P40 R41 H42 Q43 G44 VAL MET VAL GLY MET GLY Q51 K52 D53 S54 Y55 V56 E59 A60 Q61 S62 K63 R64 G65 I66 L67 T68 L69 K70 Y71 H75 D82 K86 I87
E95 V98 E101 E102 H103 P104 L107 N117 R118 M121 T122 Q123 I124 M125 F126 E127 N130 R149 H163 N164 Y168 E169 A172 L173 P174 M178 R179 L180 D181 L182 D186 L187 T188 D189 M192 K193 I194 L195 T196 E197 R198 G199 Y200 S201 F202 V203
T204 T205 A206 E207 R208 E209 I210 V211 R212 A222 L223 E228 T231 L244 P245 D246 G247 Q248 V249 I250 C259 P260 H277 M285 I289 R292 K293 Y296 A297 N298 S302 T305 Y308 M315 Q316 M327 K328 I329 K330 E336 R337 T353 F354
Q355 Q356 M357 Q362 E363 Y364 D365 E366 A367 G368 P369 S370 I371 V372 H373 R374 LYS CYS PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.19Å 75.94Å 96.75Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 24.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.4 (25.00-2.20) 91.5 (24.49-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.65 (at 2.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.233 0.185 , 0.222	Depositor DCC
R_{free} test set	2278 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 62.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8159	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.62% 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: CA, TRS, ATP, HIC

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	0.54	0/1015	0.72	0/1372
1	D	0.52	0/1008	0.69	0/1362
2	B	0.55	0/2862	0.76	2/3879 (0.1%)
2	E	0.59	0/2873	0.77	1/3894 (0.0%)
All	All	0.56	0/7758	0.75	3/10507 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	E	0	6
All	All	0	8

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	E	64	ARG	NE-CZ-NH2	-6.47	117.07	120.30
2	B	64	ARG	CD-NE-CZ	-5.85	115.42	123.60
2	B	179	ARG	CD-NE-CZ	-5.56	115.82	123.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	272	GLU	Mainchain

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Mol	Chain	Res	Type	Group
2	B	64	ARG	Sidechain
2	E	203	VAL	Peptide
2	E	210	ILE	Mainchain
2	E	285	MET	Mainchain
2	E	42	HIS	Peptide
2	E	54	SER	Mainchain
2	E	64	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	989	0	952	34	0
1	D	982	0	943	15	0
2	B	2815	0	2778	111	0
2	E	2825	0	2785	135	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
4	A	8	0	12	1	0
5	B	31	0	12	1	0
5	E	31	0	12	0	0
6	A	67	0	0	4	0
6	B	179	0	0	14	0
6	D	64	0	0	1	0
6	E	161	0	0	5	0
All	All	8159	0	7494	285	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 19.

All (285) 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:E:196:THR:HG22	2:E:201:SER:CB	1.42	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:210:ILE:HD11	2:E:244:LEU:CD2	1.63	1.28
2:E:210:ILE:CD1	2:E:244:LEU:CD2	2.27	1.13
2:E:244:LEU:HD11	2:E:250:ILE:HD11	1.11	1.10
2:E:207:GLU:HG2	2:E:211:VAL:HG23	1.25	1.09
2:E:244:LEU:HD11	2:E:250:ILE:CD1	1.86	1.06
2:E:196:THR:HG22	2:E:201:SER:HB2	1.11	1.06
2:E:196:THR:HG22	2:E:201:SER:HB3	1.33	1.05
2:E:202:PHE:HD1	2:E:202:PHE:O	1.37	1.03
2:E:196:THR:CG2	2:E:201:SER:CB	2.37	1.02
2:E:196:THR:CG2	2:E:201:SER:HB2	1.94	0.98
2:E:207:GLU:HA	2:E:210:ILE:HG22	1.43	0.97
2:E:38:GLY:O	2:E:54:SER:HB2	1.63	0.96
2:E:210:ILE:CD1	2:E:244:LEU:HD22	1.96	0.95
2:E:203:VAL:O	2:E:203:VAL:CG1	2.15	0.94
2:E:207:GLU:CA	2:E:210:ILE:HG22	1.98	0.94
2:E:244:LEU:CD1	2:E:250:ILE:HD11	1.96	0.93
2:E:207:GLU:HG2	2:E:211:VAL:CG2	1.99	0.91
2:B:258:ARG:HD2	6:B:458:HOH:O	1.69	0.91
2:E:202:PHE:HZ	2:E:244:LEU:HD12	1.37	0.89
2:B:276:ILE:HD12	2:B:315:MET:HE1	1.54	0.88
1:A:6:PRO:HA	1:A:9:LEU:HD12	1.55	0.88
2:E:210:ILE:HD11	2:E:244:LEU:HD23	1.50	0.88
2:E:39:ARG:O	2:E:67:LEU:HD12	1.74	0.87
2:B:202:PHE:HB3	2:B:207:GLU:HB3	1.56	0.86
2:E:202:PHE:O	2:E:202:PHE:CD1	2.29	0.85
2:E:195:LEU:O	2:E:200:TYR:HB2	1.75	0.85
1:D:3:VAL:HG11	2:E:353:THR:HB	1.58	0.84
2:E:222:ALA:HB1	2:E:228:GLU:HG3	1.58	0.84
2:B:227:ASN:HB3	6:B:512:HOH:O	1.75	0.84
2:E:36:ILE:HD11	2:E:71:TYR:CZ	2.12	0.83
2:B:206:ALA:O	2:B:210:ILE:HG12	1.78	0.83
2:E:207:GLU:HA	2:E:210:ILE:CG2	2.08	0.83
2:E:122:THR:OG1	2:E:372:VAL:HG11	1.78	0.82
2:E:210:ILE:HD12	2:E:244:LEU:HD22	1.61	0.82
1:A:118:LYS:H	1:A:118:LYS:HD2	1.45	0.81
2:E:201:SER:HA	2:E:207:GLU:OE1	1.82	0.80
2:E:210:ILE:HD11	2:E:244:LEU:HD21	1.59	0.80
2:E:68:THR:HG22	2:E:68:THR:O	1.81	0.79
2:E:118:ARG:HB3	2:E:118:ARG:HH11	1.47	0.79
2:B:276:ILE:HD12	2:B:315:MET:CE	2.12	0.78
2:B:61:GLN:HG2	6:B:558:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ASN:HB3	6:B:495:HOH:O	1.84	0.77
2:E:202:PHE:HZ	2:E:244:LEU:CD1	1.97	0.77
2:B:72:PRO:HG2	2:B:87:ILE:HD11	1.67	0.76
2:E:203:VAL:O	2:E:203:VAL:HG12	1.84	0.76
1:A:50:VAL:HG23	1:A:58:GLN:HG3	1.66	0.76
2:E:207:GLU:O	2:E:210:ILE:HG22	1.85	0.76
2:E:210:ILE:CD1	2:E:244:LEU:HD21	2.12	0.75
2:E:222:ALA:CB	2:E:228:GLU:HG3	2.16	0.74
2:B:258:ARG:HD3	6:B:505:HOH:O	1.87	0.74
2:E:192:MET:O	2:E:196:THR:HG23	1.87	0.74
2:B:259:CYS:HB3	2:B:260:PRO:HD3	1.70	0.73
2:E:203:VAL:O	2:E:203:VAL:HG13	1.88	0.73
2:B:192:MET:HE1	2:B:208:ARG:HG2	1.71	0.73
2:E:364:TYR:HA	2:E:371:ILE:HD11	1.71	0.73
2:B:12:CYS:HB3	2:B:107:LEU:HD23	1.71	0.73
2:E:354:PHE:HA	2:E:357:MET:HG3	1.71	0.73
1:D:37:ASP:HB3	1:D:117:LYS:HD2	1.71	0.72
1:A:50:VAL:CG2	1:A:58:GLN:HG3	2.20	0.71
2:E:210:ILE:HD12	2:E:244:LEU:CD2	2.15	0.71
2:B:204:THR:O	2:B:205:THR:OG1	2.08	0.70
2:E:118:ARG:HB3	2:E:118:ARG:NH1	2.06	0.70
2:E:201:SER:O	2:E:204:THR:HG22	1.92	0.70
2:E:36:ILE:HD11	2:E:71:TYR:CE1	2.26	0.70
2:E:202:PHE:CZ	2:E:244:LEU:CD1	2.74	0.70
2:B:74:GLU:HB2	2:B:79:THR:HG21	1.73	0.69
2:B:337:ARG:HA	2:B:340:SER:OG	1.91	0.69
2:E:207:GLU:C	2:E:210:ILE:HG22	2.13	0.69
2:E:52:LYS:HG3	2:E:53:ASP:OD1	1.93	0.68
2:E:66:ILE:HG22	2:E:66:ILE:O	1.94	0.68
2:B:99:ALA:O	2:B:102:GLU:HB2	1.93	0.68
1:A:111:LYS:H	1:A:111:LYS:HD2	1.58	0.68
1:A:2:VAL:HG11	2:B:353:THR:HB	1.76	0.68
2:B:203:VAL:HG23	6:B:582:HOH:O	1.94	0.67
2:B:354:PHE:HA	2:B:357:MET:HG3	1.77	0.66
1:A:2:VAL:HG11	2:B:353:THR:CG2	2.26	0.66
2:B:202:PHE:O	2:B:204:THR:HG23	1.96	0.66
2:B:202:PHE:HA	2:B:207:GLU:OE1	1.96	0.66
2:B:72:PRO:HG2	2:B:87:ILE:CD1	2.25	0.65
2:B:222:ALA:HB1	2:B:228:GLU:HG3	1.78	0.65
2:E:196:THR:CG2	2:E:201:SER:HB3	2.19	0.65
2:B:240:LYS:HG3	2:B:256:ARG:CZ	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:207:GLU:HG3	2:E:210:ILE:CG2	2.27	0.64
2:B:179:ARG:HD2	6:B:494:HOH:O	1.97	0.64
2:B:243:GLU:HG2	2:B:243:GLU:O	1.97	0.64
2:E:41:ARG:NH1	2:E:41:ARG:HB2	2.13	0.64
2:B:164:ASN:ND2	6:B:520:HOH:O	2.24	0.64
2:E:64:ARG:NH2	2:E:67:LEU:O	2.31	0.64
1:A:2:VAL:HG11	2:B:353:THR:HG22	1.80	0.63
1:A:2:VAL:HG11	2:B:353:THR:CB	2.29	0.63
2:B:39:ARG:HH22	2:B:86:LYS:HE2	1.64	0.62
2:E:163:HIS:NE2	2:E:179:ARG:HD3	2.14	0.62
2:E:207:GLU:O	2:E:211:VAL:HG23	1.98	0.62
2:B:202:PHE:CB	2:B:207:GLU:HB3	2.30	0.61
2:E:246:ASP:HB3	2:E:248:GLN:HG2	1.83	0.61
2:B:33:PHE:CE2	2:B:95:GLU:HG3	2.37	0.60
2:E:189:ASP:OD1	2:E:208:ARG:NH2	2.34	0.60
2:B:240:LYS:HG3	2:B:256:ARG:NH1	2.16	0.60
2:E:149:ARG:HG2	6:E:432:HOH:O	2.00	0.60
2:B:164:ASN:HB2	2:B:178:MET:HB2	1.84	0.59
2:E:293:LYS:HG2	2:E:327:MET:SD	2.42	0.59
2:B:74:GLU:HB2	2:B:79:THR:CG2	2.31	0.59
2:B:94:ASN:N	2:B:94:ASN:HD22	2.01	0.59
1:A:50:VAL:HG21	6:A:532:HOH:O	2.01	0.59
2:E:39:ARG:O	2:E:67:LEU:CD1	2.49	0.59
2:B:61:GLN:O	2:B:64:ARG:HG3	2.03	0.58
2:E:244:LEU:CD1	2:E:250:ILE:CD1	2.69	0.58
2:E:53:ASP:CG	2:E:53:ASP:O	2.41	0.58
1:A:14:GLU:HB3	2:E:316:GLN:HE22	1.69	0.58
1:D:94:GLN:NE2	2:E:169:GLU:HB3	2.18	0.58
1:D:20:TRP:HB3	1:D:27:LEU:HD22	1.85	0.58
2:E:192:MET:HG3	2:E:211:VAL:HG11	1.85	0.57
2:B:221:VAL:HG21	2:B:311:ILE:HD13	1.86	0.57
2:E:289:ILE:HA	2:E:292:ARG:HG3	1.86	0.57
2:E:182:LEU:HA	2:E:186:ASP:OD2	2.04	0.57
2:E:277:HIS:CD2	2:E:277:HIS:H	2.23	0.57
2:E:118:ARG:HH11	2:E:118:ARG:CB	2.17	0.57
1:A:112:SER:HB3	2:E:231:THR:HG23	1.87	0.57
2:E:192:MET:HG2	2:E:211:VAL:HG21	1.87	0.56
2:B:19:VAL:HG23	2:B:35:SER:HB3	1.87	0.56
1:A:15:PRO:HG3	1:A:51:GLN:HB2	1.88	0.56
2:B:222:ALA:CB	2:B:228:GLU:HG3	2.36	0.56
2:E:202:PHE:HD1	2:E:202:PHE:C	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:OD1	1:A:90:GLY:HA2	2.05	0.55
2:B:39:ARG:NH2	2:B:86:LYS:HE2	2.21	0.55
2:B:243:GLU:CD	2:B:243:GLU:H	2.08	0.55
2:B:26:ASP:OD2	2:B:30:ARG:NH1	2.40	0.55
1:A:2:VAL:HG12	1:A:2:VAL:O	2.07	0.55
2:E:36:ILE:HD11	2:E:71:TYR:CE2	2.41	0.55
2:E:207:GLU:CG	2:E:211:VAL:HG23	2.18	0.54
2:E:10:LEU:HG	2:E:103:HIS:HB3	1.88	0.54
2:E:164:ASN:HB2	2:E:178:MET:HB2	1.89	0.54
2:B:293:LYS:HG2	2:B:327:MET:SD	2.47	0.54
2:B:74:GLU:OE1	2:B:79:THR:HG21	2.07	0.54
2:E:82:ASP:O	2:E:86:LYS:HG3	2.08	0.54
2:B:204:THR:OG1	2:B:207:GLU:HB2	2.07	0.54
2:E:180:LEU:HD22	2:E:182:LEU:HB3	1.89	0.53
1:D:38:PHE:HE1	1:D:114:LEU:HD22	1.73	0.53
2:E:149:ARG:HD3	2:E:298:ASN:OD1	2.08	0.53
1:A:23:GLU:HG2	1:A:121:VAL:HG21	1.90	0.53
2:E:56:VAL:HG13	2:E:87:ILE:HD13	1.90	0.53
2:E:202:PHE:O	2:E:203:VAL:HG12	2.08	0.53
2:B:192:MET:HE1	2:B:208:ARG:HH11	1.74	0.52
2:B:9:ALA:HA	2:B:104:PRO:HD2	1.90	0.52
2:E:168:TYR:CE1	2:E:169:GLU:HG3	2.44	0.52
2:E:259:CYS:HB3	2:E:260:PRO:HD3	1.90	0.52
2:B:23:PHE:HE1	2:B:30:ARG:HD2	1.74	0.52
2:E:207:GLU:CG	2:E:210:ILE:CG2	2.88	0.51
2:B:149:ARG:HG2	6:B:415:HOH:O	2.09	0.51
2:E:202:PHE:CZ	2:E:244:LEU:HD12	2.28	0.51
2:E:202:PHE:CD1	2:E:202:PHE:C	2.78	0.51
2:B:202:PHE:CD1	2:B:202:PHE:N	2.78	0.51
2:B:277:HIS:H	2:B:277:HIS:CD2	2.28	0.51
2:E:172:ALA:O	2:E:174:PRO:HD3	2.10	0.50
2:B:192:MET:CE	2:B:208:ARG:HG2	2.41	0.50
2:E:296:TYR:CD2	2:E:327:MET:HG2	2.47	0.50
2:B:12:CYS:SG	2:B:14:ASN:ND2	2.80	0.50
2:E:187:LEU:HD23	2:E:308:TYR:OH	2.12	0.50
2:E:200:TYR:CE2	2:E:250:ILE:HG12	2.47	0.50
2:B:296:TYR:CD2	2:B:327:MET:HG2	2.47	0.50
2:B:202:PHE:O	2:B:203:VAL:C	2.50	0.49
2:B:37:VAL:HG21	2:B:83:ASP:HB3	1.95	0.49
2:E:34:PRO:O	2:E:36:ILE:N	2.44	0.49
2:E:61:GLN:C	2:E:63:LYS:N	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:PHE:CE1	2:B:30:ARG:HD2	2.46	0.49
2:E:212:ARG:HG2	2:E:212:ARG:HH11	1.77	0.49
2:B:323:ALA:HB3	2:B:329:ILE:HD11	1.94	0.49
2:B:362:GLN:O	2:B:366:GLU:HG3	2.12	0.49
1:A:72:ASP:HB3	1:A:125:PHE:CE1	2.47	0.49
2:E:61:GLN:O	2:E:63:LYS:N	2.46	0.49
2:E:207:GLU:O	2:E:211:VAL:N	2.31	0.49
1:A:51:GLN:OE1	2:E:316:GLN:HG3	2.12	0.49
2:B:101:GLU:O	2:B:132:PRO:HD3	2.13	0.49
2:B:158:GLY:O	2:B:183:ALA:HB1	2.13	0.49
1:A:111:LYS:H	1:A:111:LYS:CD	2.24	0.48
1:D:111:LYS:HG3	1:D:112:SER:N	2.28	0.48
2:B:166:PRO:HG3	2:B:283:SER:OG	2.13	0.48
2:E:12:CYS:HB3	2:E:107:LEU:HD23	1.96	0.48
2:B:151:THR:HG21	2:B:294:ASP:HB3	1.94	0.48
6:A:503:HOH:O	2:B:357:MET:HE1	2.13	0.48
2:B:149:ARG:HD3	2:B:298:ASN:OD1	2.13	0.48
2:B:362:GLN:HB2	6:B:482:HOH:O	2.13	0.48
2:E:56:VAL:CG1	2:E:87:ILE:HD13	2.44	0.47
2:E:117:ASN:O	2:E:121:MET:HG3	2.14	0.47
2:E:52:LYS:CG	2:E:52:LYS:O	2.62	0.47
2:E:302:SER:HA	2:E:337:ARG:HB2	1.96	0.47
2:E:55:TYR:HB3	2:E:59:GLU:HG2	1.95	0.47
1:D:19:ILE:HD12	1:D:35:TYR:CG	2.49	0.47
2:E:364:TYR:HE1	2:E:369:PRO:HG3	1.80	0.47
2:B:205:THR:O	2:B:209:GLU:HB2	2.16	0.46
1:A:21:ARG:NH1	1:A:121:VAL:HG23	2.30	0.46
2:B:244:LEU:HD12	2:B:248:GLN:HG2	1.96	0.46
1:D:72:ASP:HB3	1:D:125:PHE:CZ	2.51	0.46
2:E:362:GLN:O	2:E:366:GLU:HG2	2.15	0.46
2:B:151:THR:CG2	2:B:294:ASP:HB3	2.46	0.46
2:E:368:GLY:O	2:E:371:ILE:HG12	2.16	0.46
2:B:61:GLN:CG	6:B:558:HOH:O	2.54	0.46
2:B:210:ILE:HD11	2:B:245:PRO:HG3	1.97	0.46
2:E:293:LYS:NZ	6:E:548:HOH:O	2.47	0.46
2:B:64:ARG:HG2	2:B:69:LEU:HD11	1.97	0.46
2:B:109:GLU:CD	2:B:118:ARG:HE	2.18	0.46
1:A:39:PHE:HB3	1:A:119:GLY:O	2.16	0.46
2:E:10:LEU:HD11	2:E:98:VAL:HG11	1.97	0.46
1:A:118:LYS:H	1:A:118:LYS:CD	2.19	0.45
2:E:33:PHE:CE2	2:E:95:GLU:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:64:ARG:HB2	2:E:69:LEU:HD11	1.97	0.45
2:E:198:ARG:HG3	2:E:198:ARG:O	2.16	0.45
2:B:305:THR:HG22	2:B:305:THR:O	2.15	0.45
2:E:41:ARG:O	2:E:42:HIS:O	2.34	0.45
2:B:355:GLN:HG2	2:B:356:GLN:N	2.31	0.45
1:D:85:ASP:OD1	1:D:90:GLY:HA2	2.17	0.45
2:E:305:THR:HG22	2:E:305:THR:O	2.16	0.45
1:A:91:ARG:HG3	1:A:91:ARG:HH11	1.82	0.45
1:A:39:PHE:HA	1:A:117:LYS:O	2.17	0.44
2:B:356:GLN:HE21	2:B:356:GLN:HB3	1.56	0.44
1:D:3:VAL:HG22	2:E:357:MET:SD	2.57	0.44
2:B:64:ARG:HH11	2:B:64:ARG:HD2	1.61	0.44
2:B:323:ALA:HB1	2:B:324:PRO:CD	2.48	0.44
2:B:362:GLN:NE2	2:B:366:GLU:OE1	2.51	0.44
1:D:23:GLU:HG2	1:D:121:VAL:HG11	1.99	0.44
2:E:201:SER:HA	2:E:207:GLU:CD	2.37	0.43
1:D:20:TRP:CB	1:D:27:LEU:HD22	2.48	0.43
2:E:200:TYR:O	2:E:201:SER:HB3	2.18	0.43
1:A:13:LYS:NZ	6:A:519:HOH:O	2.50	0.43
2:E:228:GLU:HG2	6:E:451:HOH:O	2.18	0.43
2:B:258:ARG:CD	6:B:505:HOH:O	2.55	0.43
2:E:101:GLU:HA	2:E:130:ASN:O	2.17	0.43
2:E:123:GLN:O	2:E:127:GLU:HB2	2.19	0.43
1:A:38:PHE:HE1	1:A:114:LEU:HD22	1.84	0.43
2:B:20:LYS:HD3	2:B:20:LYS:N	2.34	0.43
1:A:94:GLN:NE2	2:B:169:GLU:HB3	2.34	0.43
2:E:53:ASP:O	2:E:53:ASP:OD2	2.37	0.43
2:B:163:HIS:CD2	2:B:179:ARG:HG3	2.54	0.43
2:B:41:ARG:HB2	2:B:68:THR:OG1	2.19	0.42
2:B:216:GLU:HG2	5:B:400:ATP:C4	2.54	0.42
2:B:367:ALA:HB3	2:B:371:ILE:HG21	2.01	0.42
2:B:61:GLN:CD	6:B:558:HOH:O	2.57	0.42
2:B:289:ILE:O	2:B:289:ILE:HG13	2.19	0.42
2:B:98:VAL:HB	2:B:103:HIS:CE1	2.54	0.42
2:E:195:LEU:HD12	2:E:195:LEU:HA	1.81	0.42
2:B:51:GLN:HG3	2:B:52:LYS:N	2.34	0.42
2:B:168:TYR:CE1	2:B:169:GLU:HG3	2.53	0.42
2:B:360:THR:OG1	2:B:363:GLU:HG3	2.18	0.42
2:E:207:GLU:CA	2:E:210:ILE:CG2	2.78	0.42
2:B:240:LYS:CG	2:B:256:ARG:NH1	2.81	0.42
2:E:207:GLU:CG	2:E:211:VAL:CG2	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:HH11	1:A:53:ARG:HG3	1.85	0.42
2:B:202:PHE:HB2	2:B:203:VAL:H	1.62	0.42
2:E:41:ARG:HB2	2:E:41:ARG:HH11	1.84	0.42
4:A:472:TRS:H32	6:E:454:HOH:O	2.18	0.42
2:E:61:GLN:C	2:E:63:LYS:H	2.22	0.42
2:E:64:ARG:CZ	2:E:67:LEU:O	2.68	0.42
2:B:92:PHE:CG	2:B:100:PRO:HG3	2.55	0.42
2:E:123:GLN:HG3	2:E:124:ILE:N	2.35	0.42
2:B:192:MET:CE	2:B:208:ARG:HH11	2.33	0.42
2:B:355:GLN:CG	2:B:356:GLN:N	2.82	0.42
1:A:53:ARG:HG3	1:A:53:ARG:NH1	2.36	0.41
2:B:222:ALA:HB1	2:B:228:GLU:CG	2.49	0.41
2:B:277:HIS:CE1	2:B:278:GLU:HG3	2.55	0.41
2:B:193:LYS:NZ	6:B:545:HOH:O	2.54	0.41
1:D:96:ARG:NH1	6:D:427:HOH:O	2.40	0.41
1:D:9:LEU:HD23	1:D:87:TYR:OH	2.21	0.41
2:E:293:LYS:HG3	6:E:463:HOH:O	2.20	0.41
1:A:41:GLY:HA2	1:A:68:GLU:HB2	2.03	0.41
2:B:161:VAL:HG22	2:B:162:THR:N	2.36	0.41
1:A:79:ILE:O	1:A:83:GLN:HG3	2.20	0.41
2:B:311:ILE:HG23	2:B:312:ALA:N	2.36	0.41
2:E:103:HIS:HA	2:E:104:PRO:HD3	1.93	0.41
2:B:100:PRO:HD2	2:B:101:GLU:OE1	2.20	0.41
2:B:254:ASN:HA	2:B:257:PHE:CE2	2.56	0.41
2:B:355:GLN:HE21	2:B:355:GLN:HB3	1.54	0.41
2:E:101:GLU:H	2:E:101:GLU:CD	2.23	0.41
2:E:126:PHE:O	2:E:130:ASN:HA	2.20	0.41
6:A:534:HOH:O	2:E:223:LEU:HD23	2.19	0.41
2:B:153:ILE:HG23	2:B:153:ILE:O	2.21	0.41
2:E:369:PRO:O	2:E:372:VAL:HG22	2.21	0.41
1:A:38:PHE:CE1	1:A:114:LEU:HD22	2.57	0.40
2:B:51:GLN:OE1	2:B:53:ASP:HB2	2.21	0.40
2:E:19:VAL:O	2:E:32:VAL:HA	2.21	0.40
1:A:27:LEU:HD23	1:A:27:LEU:HA	1.91	0.40
1:A:121:VAL:HG12	1:A:122:ALA:N	2.37	0.40
2:B:276:ILE:HD12	2:B:315:MET:HE2	1.99	0.40
1:D:37:ASP:OD1	1:D:115:LYS:HB3	2.22	0.40
2:E:194:ILE:HD13	2:E:194:ILE:HG21	1.84	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	122/125 (98%)	114 (93%)	8 (7%)	0	100	100
1	D	121/125 (97%)	117 (97%)	4 (3%)	0	100	100
2	B	356/377 (94%)	338 (95%)	17 (5%)	1 (0%)	41	46
2	E	357/377 (95%)	333 (93%)	17 (5%)	7 (2%)	7	4
All	All	956/1004 (95%)	902 (94%)	46 (5%)	8 (1%)	19	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	52	LYS
2	E	42	HIS
2	E	246	ASP
2	B	205	THR
2	E	101	GLU
2	E	53	ASP
2	E	65	GLY
2	E	203	VAL

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	102/103 (99%)	98 (96%)	4 (4%)	32	41
1	D	101/103 (98%)	95 (94%)	6 (6%)	19	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	303/319 (95%)	287 (95%)	16 (5%)	22	27
2	E	304/319 (95%)	279 (92%)	25 (8%)	11	11
All	All	810/844 (96%)	759 (94%)	51 (6%)	18	20

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	53	ARG
1	A	58	GLN
1	A	118	LYS
2	B	30	ARG
2	B	41	ARG
2	B	51	GLN
2	B	94	ASN
2	B	149	ARG
2	B	202	PHE
2	B	203	VAL
2	B	208	ARG
2	B	249	VAL
2	B	251	THR
2	B	289	ILE
2	B	336	GLU
2	B	355	GLN
2	B	356	GLN
2	B	357	MET
2	B	361	LYS
1	D	27	LEU
1	D	32	THR
1	D	52	LEU
1	D	53	ARG
1	D	63	TYR
1	D	68	GLU
2	E	41	ARG
2	E	43	GLN
2	E	52	LYS
2	E	53	ASP
2	E	63	LYS
2	E	64	ARG
2	E	68	THR
2	E	118	ARG

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Mol	Chain	Res	Type
2	E	123	GLN
2	E	180	LEU
2	E	195	LEU
2	E	198	ARG
2	E	202	PHE
2	E	203	VAL
2	E	205	THR
2	E	210	ILE
2	E	315	MET
2	E	316	GLN
2	E	328	LYS
2	E	330	LYS
2	E	336	GLU
2	E	355	GLN
2	E	356	GLN
2	E	357	MET
2	E	366	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	61	GLN
2	B	94	ASN
2	B	103	HIS
2	B	130	ASN
2	B	277	HIS
2	B	355	GLN
2	B	356	GLN
1	D	33	ASN
1	D	51	GLN
1	D	67	ASN
2	E	61	GLN
2	E	89	HIS
2	E	94	ASN
2	E	123	GLN
2	E	227	ASN
2	E	277	HIS
2	E	316	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)

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	$\#\|Z\| > 2$
2	HIC	B	75	2	8,11,12	2.89	1 (12%)	6,14,16	1.10	0
2	HIC	E	75	2	8,11,12	4.66	2 (25%)	6,14,16	1.60	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIC	B	75	2	-	0/5/6/8	0/1/1/1
2	HIC	E	75	2	-	0/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	75	HIC	CZ-NE2	-12.83	1.13	1.48
2	B	75	HIC	CZ-NE2	-7.94	1.26	1.48
2	E	75	HIC	CD2-CG	2.55	1.40	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	75	HIC	CZ-NE2-CD2	3.23	137.53	126.31
2	E	75	HIC	CZ-NE2-CE1	-2.04	115.51	125.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
5	ATP	B	400	3	26,33,33	2.15	9 (34%)	31,52,52	2.90	8 (25%)
4	TRS	A	472	-	7,7,7	1.13	1 (14%)	9,9,9	2.25	4 (44%)
5	ATP	E	400	3	26,33,33	1.96	8 (30%)	31,52,52	2.81	8 (25%)

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
5	ATP	B	400	3	-	1/18/38/38	0/3/3/3
4	TRS	A	472	-	-	6/9/9/9	-
5	ATP	E	400	3	-	1/18/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	400	ATP	C4-N3	6.27	1.44	1.35
5	B	400	ATP	C4-N3	5.90	1.43	1.35
5	B	400	ATP	C8-N7	-3.94	1.27	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	400	ATP	O5'-C5'	-3.36	1.31	1.44
5	B	400	ATP	O4'-C1'	3.24	1.45	1.41
5	E	400	ATP	O5'-C5'	-3.10	1.32	1.44
5	B	400	ATP	C2-N3	2.95	1.36	1.32
5	E	400	ATP	C8-N7	-2.80	1.29	1.34
5	B	400	ATP	PA-O5'	-2.64	1.48	1.59
5	E	400	ATP	PB-O2B	-2.54	1.43	1.55
5	E	400	ATP	O4'-C1'	2.45	1.44	1.41
5	B	400	ATP	PA-O1A	-2.29	1.42	1.50
5	E	400	ATP	PA-O1A	-2.29	1.42	1.50
5	B	400	ATP	PB-O2B	-2.23	1.44	1.55
5	E	400	ATP	PA-O5'	-2.21	1.50	1.59
5	E	400	ATP	C5-C4	-2.11	1.35	1.40
5	B	400	ATP	C5-C4	-2.06	1.35	1.40
4	A	472	TRS	C-N	-2.03	1.42	1.49

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	400	ATP	O5'-C5'-C4'	11.11	147.21	108.99
5	E	400	ATP	O5'-C5'-C4'	10.70	145.81	108.99
5	B	400	ATP	O5'-PA-O1A	-6.69	82.95	109.07
5	E	400	ATP	O5'-PA-O1A	-6.49	83.72	109.07
5	E	400	ATP	PA-O5'-C5'	5.32	152.85	121.68
5	B	400	ATP	PA-O5'-C5'	5.02	151.15	121.68
4	A	472	TRS	O1-C1-C	-3.73	99.17	111.00
5	B	400	ATP	O4'-C4'-C3'	3.44	111.92	105.11
5	B	400	ATP	C3'-C2'-C1'	3.24	105.85	100.98
5	E	400	ATP	C1'-N9-C4	-3.16	121.09	126.64
5	B	400	ATP	C5'-C4'-C3'	-3.13	103.43	115.18
5	B	400	ATP	C1'-N9-C4	-2.91	121.52	126.64
5	E	400	ATP	O4'-C4'-C3'	2.91	110.87	105.11
4	A	472	TRS	C2-C-N	2.90	116.64	107.98
4	A	472	TRS	C2-C-C1	-2.89	101.86	110.81
5	E	400	ATP	C3'-C2'-C1'	2.67	105.00	100.98
4	A	472	TRS	C3-C-N	2.63	115.82	107.98
5	E	400	ATP	C5'-C4'-C3'	-2.62	105.35	115.18
5	E	400	ATP	C4-C5-N7	2.42	111.92	109.40
5	B	400	ATP	O2A-PA-O1A	2.08	122.54	112.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	472	TRS	C2-C-C1-O1
4	A	472	TRS	C3-C-C1-O1
4	A	472	TRS	N-C-C1-O1
4	A	472	TRS	C1-C-C3-O3
4	A	472	TRS	C2-C-C3-O3
5	B	400	ATP	PG-O3B-PB-O2B
5	E	400	ATP	PG-O3B-PB-O2B
4	A	472	TRS	N-C-C3-O3

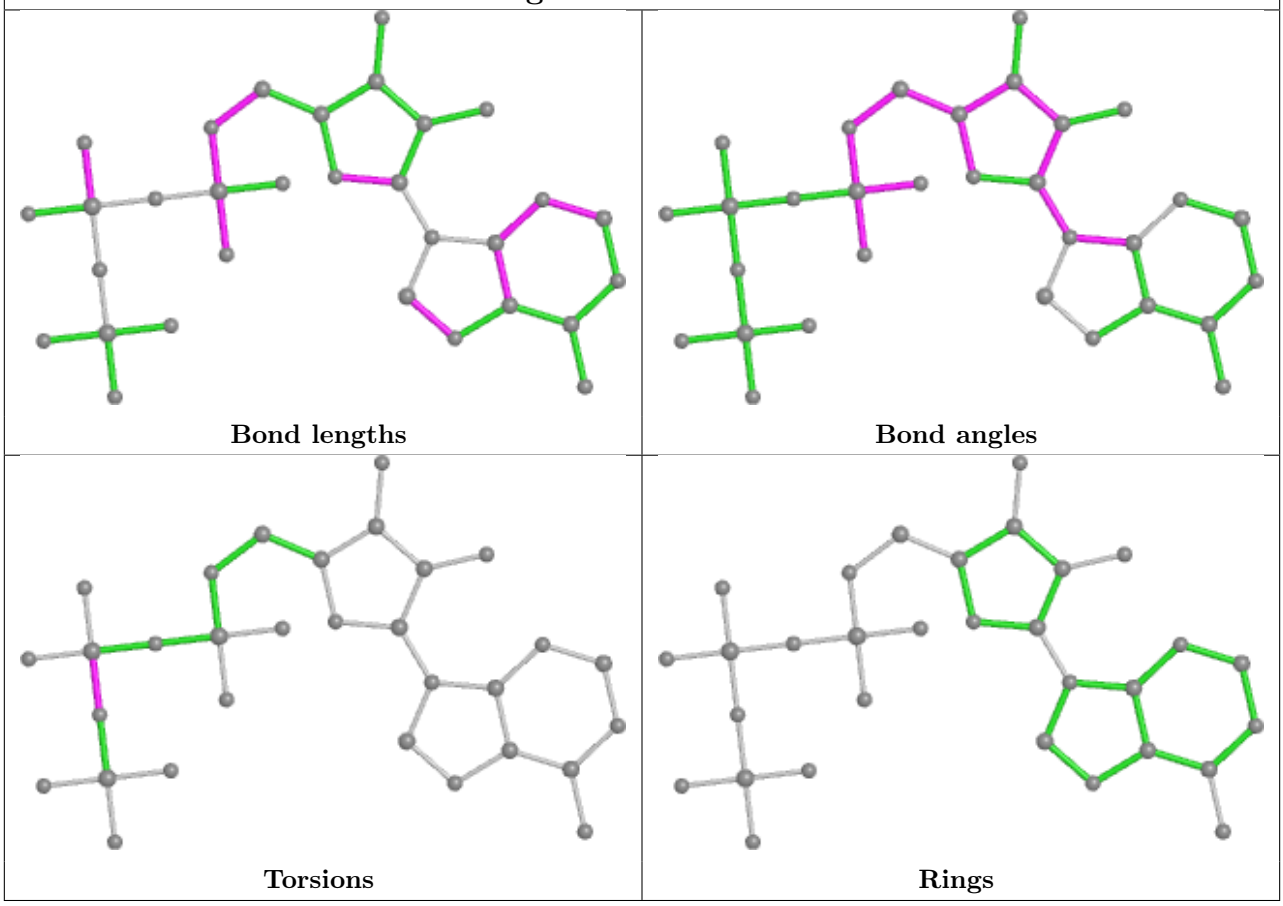
There are no ring outliers.

2 monomers are involved in 2 short contacts:

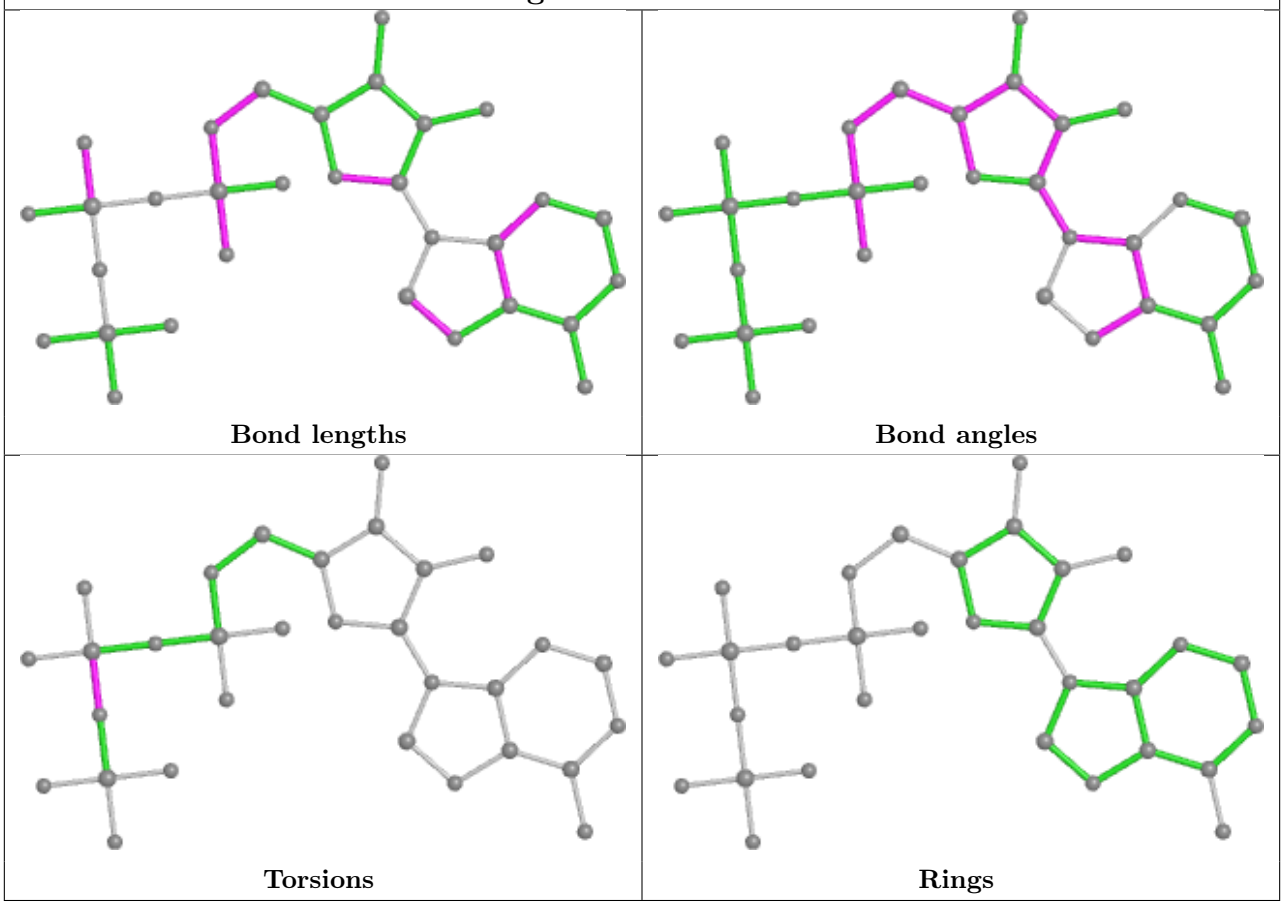
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	400	ATP	1	0
4	A	472	TRS	1	0

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 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 ATP B 400



Ligand ATP E 400



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	124/125 (99%)	0.04	4 (3%)	47	45	19, 37, 52, 60	0
1	D	123/125 (98%)	-0.08	4 (3%)	46	44	21, 34, 52, 60	0
2	B	360/377 (95%)	-0.08	14 (3%)	39	37	15, 32, 59, 60	0
2	E	361/377 (95%)	0.09	26 (7%)	15	14	14, 30, 60, 60	0
All	All	968/1004 (96%)	-0.00	48 (4%)	28	27	14, 32, 60, 60	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	VAL	10.5
2	E	44	GLY	8.3
1	A	3	VAL	8.1
2	E	65	GLY	7.0
2	E	204	THR	6.2
2	E	43	GLN	6.1
2	E	201	SER	5.7
2	E	64	ARG	5.6
2	B	205	THR	5.6
2	B	204	THR	5.4
2	E	205	THR	5.4
2	E	66	ILE	5.1
2	B	245	PRO	4.8
2	E	40	PRO	4.5
2	E	42	HIS	4.4
2	E	51	GLN	4.1
2	E	41	ARG	4.0
2	E	62	SER	4.0
2	B	375	LYS	4.0
2	E	7	THR	4.0
2	E	203	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
2	E	245	PRO	3.8
2	B	203	VAL	3.6
2	B	272	GLU	3.5
2	E	206	ALA	3.4
1	D	4	GLU	3.4
2	B	7	THR	3.3
2	E	52	LYS	3.2
2	E	39	ARG	3.0
2	E	207	GLU	3.0
2	B	247	GLY	2.9
1	A	4	GLU	2.9
2	B	50	GLY	2.9
1	D	3	VAL	2.8
2	E	54	SER	2.8
1	D	45	VAL	2.7
2	B	101	GLU	2.6
2	B	356	GLN	2.5
2	E	200	TYR	2.4
2	B	106	LEU	2.4
2	E	370	SER	2.3
2	E	373	HIS	2.3
2	E	374	ARG	2.3
1	D	9	LEU	2.3
2	B	362	GLN	2.3
2	E	38	GLY	2.2
1	A	104	ALA	2.2
2	B	243	GLU	2.1

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
2	HIC	B	75	11/12	0.95	0.10	22,31,47,48	0
2	HIC	E	75	11/12	0.96	0.11	24,31,42,45	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

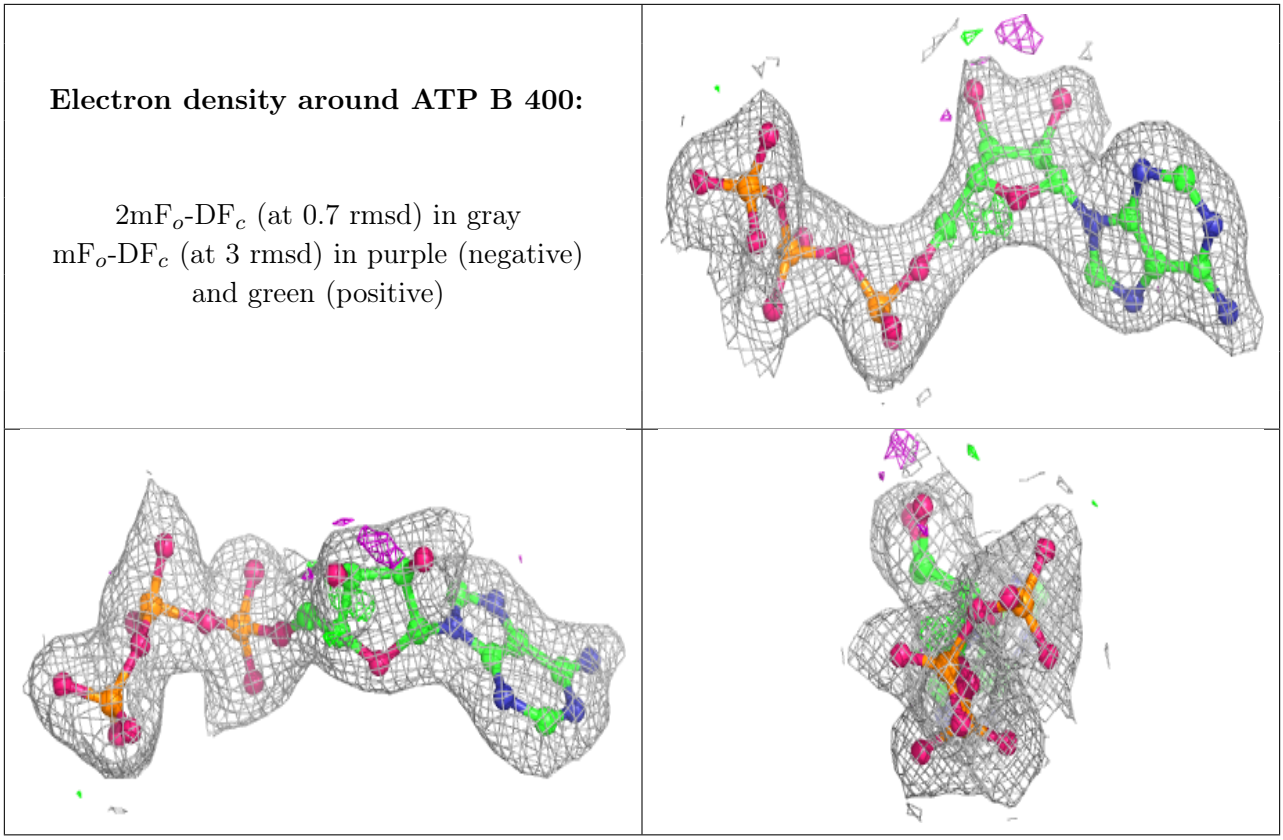
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TRS	A	472	8/8	0.72	0.23	54,60,60,60	0
3	CA	B	404	1/1	0.96	0.11	50,50,50,50	0
3	CA	A	402	1/1	0.97	0.05	43,43,43,43	0
5	ATP	B	400	31/31	0.97	0.10	17,24,30,34	0
3	CA	B	401	1/1	0.98	0.10	29,29,29,29	0
5	ATP	E	400	31/31	0.98	0.09	17,24,28,29	0
3	CA	D	403	1/1	0.99	0.04	24,24,24,24	0
3	CA	D	402	1/1	0.99	0.03	36,36,36,36	0
3	CA	E	401	1/1	1.00	0.11	29,29,29,29	0
3	CA	A	403	1/1	1.00	0.05	25,25,25,25	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.

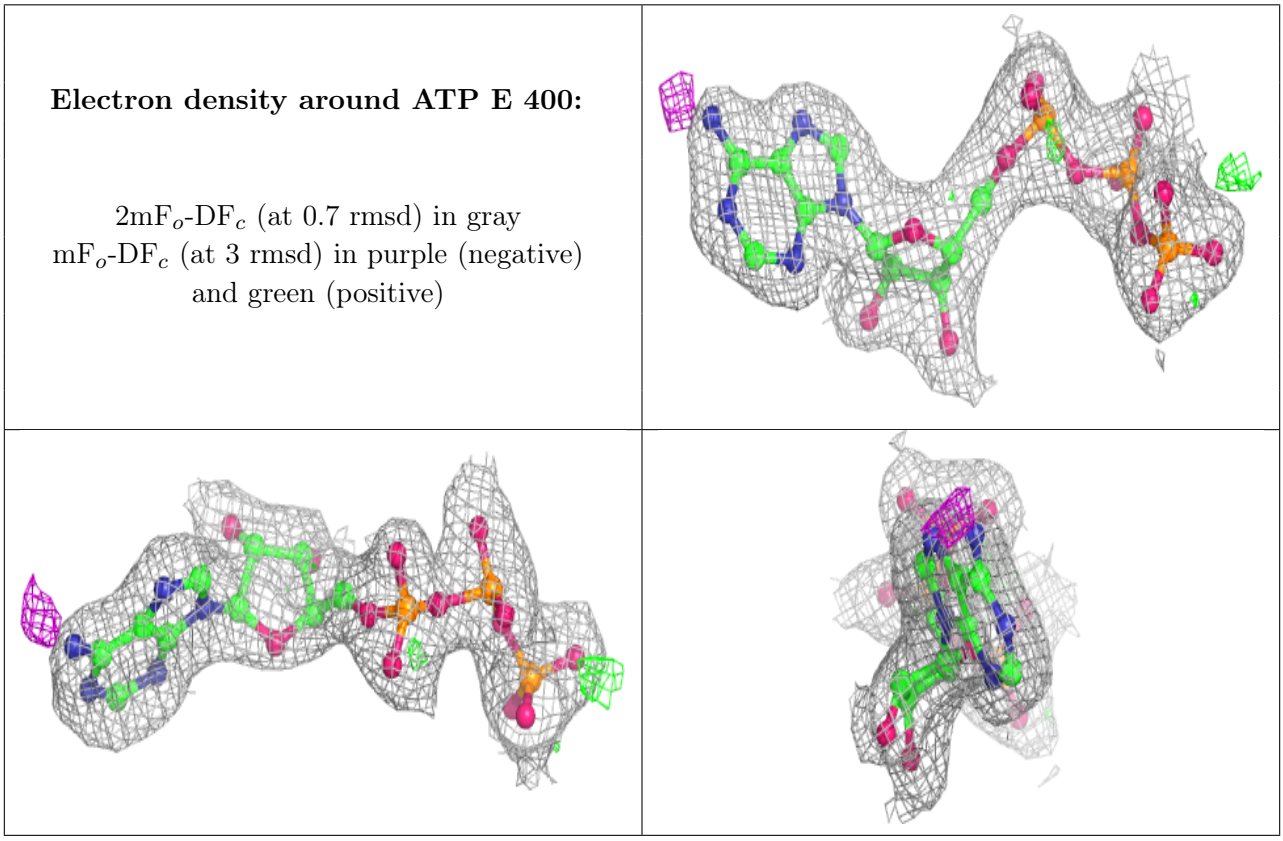
Electron density around ATP B 400:

$2mF_o$-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 E 400:

$2mF_o$-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.