



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:38 AM GMT

PDB ID : 3FFK
Title : Crystal structure of human Gelsolin domains G1-G3 bound to Actin
Authors : Chumnarnsilpa, S.; Robinson, R.C.; Burtneck, 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

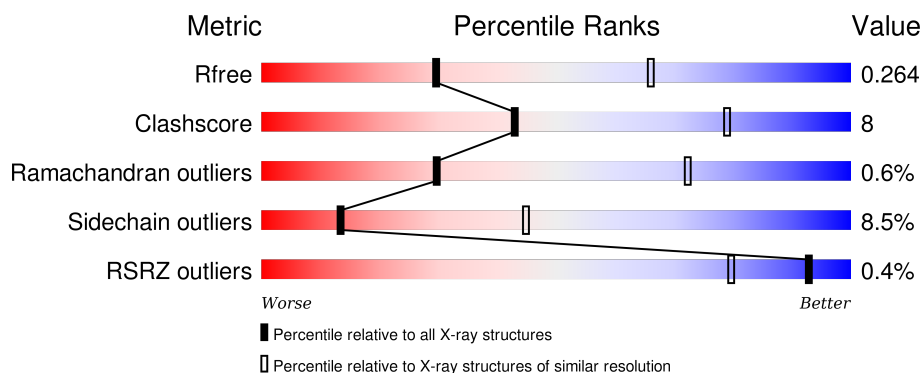
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>74%</div> <div>17%</div> <div>8%</div> </div>
1	D	377	<div> <div>72%</div> <div>17%</div> <div>8%</div> </div>
2	B	377	<div> <div>%</div> <div>77%</div> <div>17%</div> <div>•</div> <div>•</div> </div>
2	E	377	<div> <div>73%</div> <div>18%</div> <div>6%</div> </div>

2 Entry composition

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
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

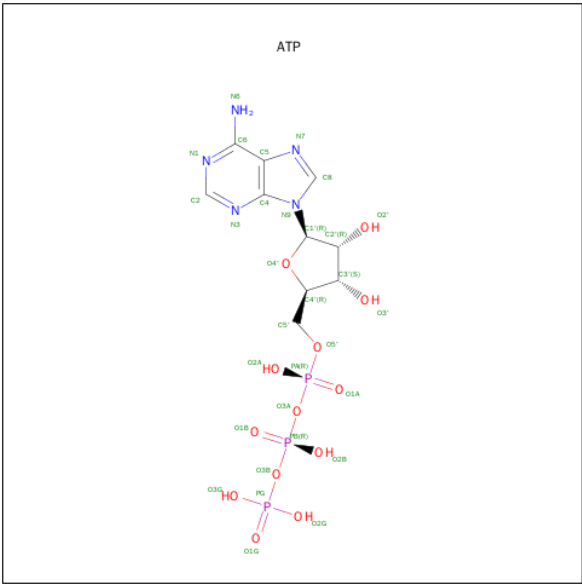
- Molecule 2 is a protein called actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 (three-letter code: CA) (formula: Ca).

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

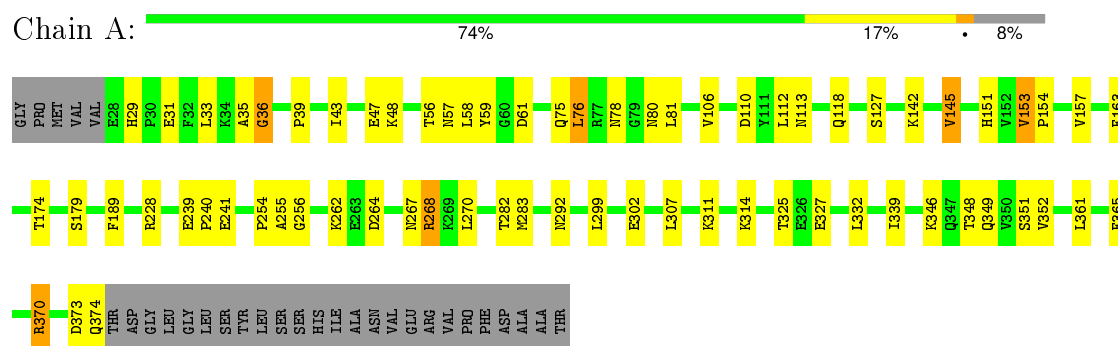
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



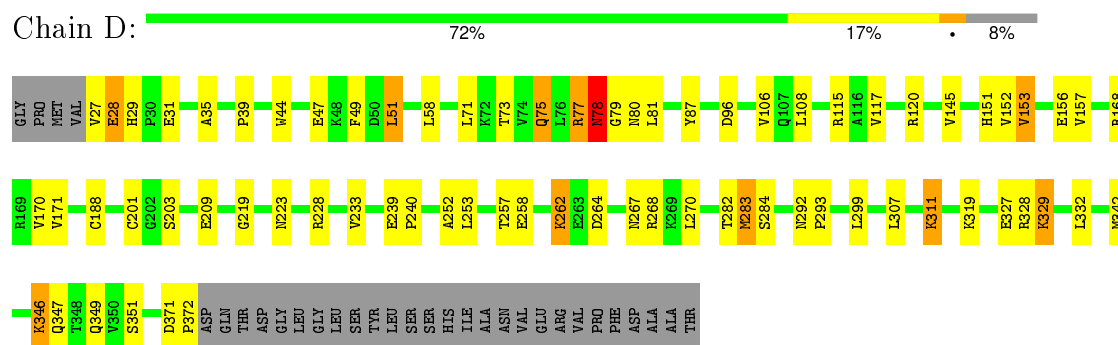
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

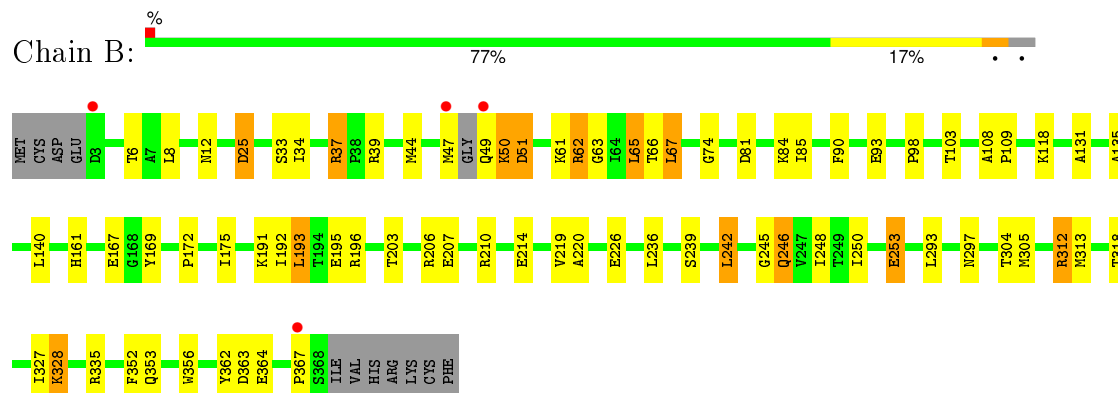
- Molecule 1: plasma gelsolin




- Molecule 1: plasma gelsolin



- Molecule 2: actin, alpha skeletal muscle



- Chain E: 
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| MET | CYS | ASP | GLU | ASP | GLU | T5 | N12 | K18 | A19 | G20 | D26 | Y36 | G36 | R37 | ARG | HIS | GLN | GLY | VAL | MET | GLY | GLY | GLN | K50 | D51 | G63 | I64 | L65 | T66 | I75 | D81 | K84 | I85 | W86 | E93 | E100 | L104 | N111 | P112 | N115 | A131 | | | | | |
| G156 | L180 | A181 | G182 | L185 | M190 | K191 | I192 | L193 | T194 | E195 | R196 | F200 | V201 | T202 | T203 | A204 | E205 | R206 | E207 | L208 | V209 | R210 | K213 | E214 | C217 | V218 | L219 | A220 | L221 | D222 | N225 | E226 | L236 | D244 | T249 | L250 | E253 | R254 | F255 | R256 | C257 | P258 | E259 | T260 | E270 | S271 |
| L293 | N297 | T303 | T304 | R312 | P322 | S323 | T324 | P332 | R335 | L346 | A347 | S350 | T351 | F352 | Q353 | W356 | G366 | I369 | V370 | HIS | ARG | LYS | CYS | PHE | | | | | | | | | | | | | | | | | | | | | | |

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 28.05 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.00) 99.8 (28.05-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.201 , 0.273 0.196 , 0.264	Depositor DCC
R_{free} test set	2264 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.7	EDS
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 45217 reflections (0.002%)	Xtriage
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

Xtriage'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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/2841	0.62	1/3834 (0.0%)
1	D	0.45	0/2802	0.59	1/3785 (0.0%)
2	B	0.46	0/2906	0.59	0/3938
2	E	0.45	0/2838	0.61	1/3849 (0.0%)
All	All	0.45	0/11387	0.60	3/15406 (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
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	65	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	36	GLY	N-CA-C	-5.57	99.18	113.10
1	D	78	ASN	N-CA-C	5.55	125.98	111.00

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 ⓘ

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	43	0
1	D	2737	0	2691	46	0
2	B	2846	0	2808	51	0
2	E	2779	0	2749	54	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	1	0
5	D	103	0	0	2	0
5	E	126	0	0	7	0
All	All	11677	0	11002	183	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 8.

All (183) 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
2:B:37:ARG:HH11	2:B:37:ARG:HG2	1.33	0.92
1:D:311:LYS:CD	1:D:311:LYS:H	1.82	0.92
2:B:245:GLY:HA3	2:B:246:GLN:HB3	1.50	0.89
1:D:311:LYS:N	1:D:311:LYS:HD2	1.88	0.89
1:D:283:MET:HE1	1:D:327:GLU:HA	1.55	0.89
2:E:37:ARG:HG2	2:E:37:ARG:HH11	1.39	0.88
1:A:311[B]:LYS:H	1:A:311[B]:LYS:HD2	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:NZ	1:D:262:LYS:HB3	1.97	0.77
1:A:118:GLN:CD	2:B:167:GLU:HG3	2.04	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:D:188:CYS:HG	1:D:201:CYS:HG	0.76	0.72
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: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:HA	2:E:270:GLU:OE2	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:N	1:D:311:LYS:CD	2.54	0.64
1:D:44:TRP:CB	1:D:51:LEU:HD22	2.29	0.62
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:352:PHE:HE2	2:E:356:TRP:CZ3	2.18	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
1:D:44:TRP:HB3	1:D:51:LEU:HD22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	1:A:311[B]:LYS:HD2	2.16	0.58
1:A:268:ARG:CD	1:A:292:ASN:O	2.52	0.58
2:B:37:ARG:NH1	2:B:37:ARG:HG2	2.11	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:262:LYS:HB3	1:D:262:LYS:HZ3	1.68	0.56
1:D:27:VAL:HG23	1:D:28:GLU:H	1.69	0.56
1:D:283:MET:CE	1:D:327:GLU:HA	2.34	0.55
1:D:346:LYS:O	1:D:347:GLN:HB2	2.05	0.55
1:A:283:MET:HE1	1:A:327:GLU:HG3	1.87	0.55
2:E:51:ASP:HB3	5:E:418:HOH:O	2.07	0.55
1:D:77:ARG:HA	1:D:78:ASN:C	2.26	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: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
2:E:253:GLU:HA	2:E:256:ARG:HB2	1.91	0.52
1:D:171:VAL:HG11	1:D:209:GLU:HA	1.91	0.52
2:E:218:TYR:O	2:E:255:PHE:HA	2.10	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:250:ILE:HG13	2:E:253:GLU:CG	2.43	0.48
1:D:170:VAL:HG21	1:D:268:ARG:HD3	1.94	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
2:E:347:ALA:HA	2:E:352:PHE:CD2	2.49	0.47
1:D:87:TYR:CE1	1:D:120:ARG:HG3	2.50	0.47
2:E:332:PRO:O	2:E:335:ARG:HB3	2.15	0.47
1:A:39:PRO:HG3	1:A:75:GLN:HB2	1.96	0.47
2:B:352:PHE:CE2	2:B:356:TRP:CH2	3.00	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
1:D:371:ASP:HA	1:D:372:PRO:HD2	1.69	0.46
1:D:239:GLU:HA	1:D:240:PRO:HD3	1.77	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:B:49:GLN:CG	2:B:50:LYS:H	2.21	0.46
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
2:B:193:LEU:HD11	2:B:250:ILE:HD12	1.99	0.45
2:B:172:PRO:HA	2:B:175: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
2:B:37:ARG:NH2	2:B:81:ASP:OD1	2.44	0.44
1:A:339:ILE:HG21	1:A:346[B]:LYS:HE2	2.00	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:B:226:GLU:OE1	2:B:236:LEU:HD21	2.18	0.43
1:A:370:ARG:HB2	1:A:370:ARG:HE	1.66	0.43
2:E:214:GLU:HB2	4:E:380:ATP:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:PRO:HG3	1:D:75:GLN:HB2	2.00	0.43
2:B:74:GLY:O	2:B:108:ALA:HB2	2.19	0.43
1:D:328:ARG:HD3	2:E:100:GLU:OE1	2.18	0.43
2:E:192:ILE:HA	2:E:192:ILE:HD12	1.79	0.43
1:A:239:GLU:HA	1:A:240:PRO:HD3	1.81	0.43
1:A:268:ARG:HD2	1:A:292:ASN:O	2.19	0.43
2:E:353[B]:GLN:HA	2:E:356:TRP:NE1	2.34	0.43
2:E:203:THR:HG22	2:E:206:ARG:NH2	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
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
1:A:43:ILE:HD12	1:A:59:TYR:CG	2.54	0.42
2:B:362:TYR:C	2:B:364:GLU:H	2.22	0.42
2:B:242:LEU:HD12	2:B:246:GLN:O	2.20	0.42
1:D:262:LYS:HZ2	1:D:262:LYS:HB3	1.79	0.42
1:D:371:ASP:N	1:D:371:ASP:OD1	2.53	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:153:VAL:HA	1:A:154:PRO:HD3	1.90	0.42
2:E:156:GLY:O	2:E:181:ALA:HB1	2.20	0.42
2:B:318:THR:HA	2:B:327:ILE:HD13	2.02	0.42
1:A:163:PHE:O	1:A:189:PHE:HA	2.20	0.42
1:A:314:LYS:HE3	1:A:361:LEU:HD13	2.01	0.41
2:E:20:GLY:HA3	5:E:423:HOH:O	2.19	0.41
2:B:109:PRO:HG2	2:B:161:HIS:CD2	2.54	0.41
2:E:222:ASP:OD1	2:E:222:ASP:C	2.59	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:NH1	2:E:37:ARG:CG	2.65	0.41
1:A:47:GLU:HG2	1:A:145:VAL:HG11	2.01	0.41
1:D:49:PHE:CE2	1:D:96:ASP:HB2	2.56	0.41
2:E:222:ASP:CG	2:E:225:ASN:HD22	2.24	0.41
2:E:180:LEU:HD11	2:E:260:THR:HG22	2.03	0.41
1:D:168:ARG:HB3	1:D:264:ASP:OD2	2.21	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:D:29:HIS:HD2	1:D:31:GLU:H	1.66	0.41
1:A:47:GLU:O	1:A:48:LYS:C	2.59	0.41
2:E:257:CYS:HB3	2:E:258:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:111:ASN:HA	2:E:112:PRO:HD3	1.94	0.41
1:A:283:MET:HE1	1:A:327:GLU:CG	2.51	0.40
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%)	30	72
2	B	361/377 (96%)	344 (95%)	13 (4%)	4 (1%)	17	58
2	E	352/377 (93%)	334 (95%)	15 (4%)	3 (1%)	21	64
All	All	1407/1508 (93%)	1328 (94%)	70 (5%)	9 (1%)	30	72

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 ⓘ

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%)	264 (90%)	30 (10%)	9	33
1	D	290/314 (92%)	263 (91%)	27 (9%)	11	39
2	B	308/320 (96%)	286 (93%)	22 (7%)	18	54
2	E	302/320 (94%)	279 (92%)	23 (8%)	16	51
All	All	1194/1268 (94%)	1092 (92%)	102 (8%)	13	45

All (102) 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
1	A	61	ASP
1	A	76	LEU
1	A	81	LEU
1	A	106	VAL
1	A	112	LEU
1	A	113	ASN
1	A	127	SER
1	A	142	LYS
1	A	145	VAL
1	A	153	VAL
1	A	157	VAL
1	A	174	THR
1	A	179	SER
1	A	241	GLU
1	A	262	LYS
1	A	264	ASP
1	A	268	ARG
1	A	282	THR
1	A	299	LEU
1	A	302	GLU
1	A	307	LEU

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Mol	Chain	Res	Type
1	A	325	THR
1	A	332	LEU
1	A	349	GLN
1	A	351	SER
1	A	352	VAL
1	A	370	ARG
2	B	6	THR
2	B	12	ASN
2	B	25	ASP
2	B	33	SER
2	B	37	ARG
2	B	44	MET
2	B	47	MET
2	B	51	ASP
2	B	62	ARG
2	B	65	LEU
2	B	67	LEU
2	B	84	LYS
2	B	85	ILE
2	B	118	LYS
2	B	193	LEU
2	B	239	SER
2	B	242	LEU
2	B	253	GLU
2	B	293	LEU
2	B	312	ARG
2	B	313	MET
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	117	VAL
1	D	152	VAL
1	D	153	VAL
1	D	157	VAL
1	D	203	SER
1	D	233	VAL

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Mol	Chain	Res	Type
1	D	262	LYS
1	D	282	THR
1	D	283	MET
1	D	284	SER
1	D	299	LEU
1	D	307	LEU
1	D	311	LYS
1	D	329	LYS
1	D	332	LEU
1	D	342	MET
1	D	346	LYS
1	D	349	GLN
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	84	LYS
2	E	115	ASN
2	E	185	LEU
2	E	190	MET
2	E	192	ILE
2	E	193	LEU
2	E	196	ARG
2	E	236	LEU
2	E	244	ASP
2	E	253	GLU
2	E	271	SER
2	E	293	LEU
2	E	297	ASN
2	E	312	ARG
2	E	353[A]	GLN
2	E	353[B]	GLN
2	E	370	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	75	GLN

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Mol	Chain	Res	Type
1	A	78	ASN
1	A	151	HIS
1	A	195	ASN
1	A	232	HIS
1	A	267	ASN
1	A	347	GLN
2	B	73	HIS
2	B	128	ASN
2	B	161	HIS
2	B	263	GLN
2	B	280	ASN
1	D	29	HIS
1	D	113	ASN
1	D	151	HIS
1	D	160	GLN
1	D	196	ASN
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	121	GLN
2	E	225	ASN
2	E	280	ASN
2	E	354	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates 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	B	380	3	24,33,33	0.92	1 (4%)	31,52,52	1.94	6 (19%)
4	ATP	E	380	3	24,33,33	0.99	1 (4%)	31,52,52	1.89	6 (19%)

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	B	380	3	-	0/18/38/38	0/3/3/3
4	ATP	E	380	3	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	380	ATP	C5-C4	3.09	1.47	1.40
4	B	380	ATP	C5-C4	3.17	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	380	ATP	N3-C2-N1	-7.33	123.28	128.89
4	E	380	ATP	N3-C2-N1	-6.43	123.97	128.89
4	E	380	ATP	PA-O3A-PB	-4.22	120.89	132.73
4	B	380	ATP	PA-O3A-PB	-3.27	123.54	132.73
4	B	380	ATP	C4-C5-N7	-3.15	106.58	109.48
4	E	380	ATP	C4-C5-N7	-3.03	106.69	109.48
4	B	380	ATP	C1'-N9-C4	-2.86	122.62	126.94
4	E	380	ATP	PB-O3B-PG	-2.46	124.42	132.67
4	B	380	ATP	PB-O3B-PG	-2.25	125.11	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	380	ATP	C2'-C1'-N9	-2.04	111.17	114.29
4	B	380	ATP	C2'-C1'-N9	-2.03	111.19	114.29
4	E	380	ATP	O4'-C1'-N9	3.03	114.44	108.10

There are no chirality outliers.

There are no torsion outliers.

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

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%)	-0.56	0	100 100	17, 29, 48, 58	0
1	D	346/377 (91%)	-0.58	0	100 100	10, 19, 33, 53	0
2	B	365/377 (96%)	-0.51	4 (1%)	82 58	7, 16, 33, 57	0
2	E	355/377 (94%)	-0.65	1 (0%)	94 84	8, 17, 30, 37	0
All	All	1413/1508 (93%)	-0.58	5 (0%)	93 80	7, 19, 41, 58	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	49	GLN	3.1
2	B	3	ASP	2.9
2	B	47	MET	2.6
2	E	201	VAL	2.2
2	B	367	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å ²)	Q<0.9
3	CA	A	757	1/1	0.96	0.12	-0.19	8,8,8,8	0
4	ATP	B	380	31/31	0.99	0.15	-0.24	7,10,14,14	0
4	ATP	E	380	31/31	0.98	0.14	-0.29	13,18,21,22	0
3	CA	E	401	1/1	0.99	0.14	-0.38	18,18,18,18	0
3	CA	A	756	1/1	0.96	0.10	-1.41	3,3,3,3	0
3	CA	A	758	1/1	0.90	0.07	-1.46	15,15,15,15	0
3	CA	D	758	1/1	0.97	0.07	-1.85	31,31,31,31	0
3	CA	D	757	1/1	0.99	0.07	-1.88	28,28,28,28	0
3	CA	D	759	1/1	0.98	0.05	-2.70	26,26,26,26	0
3	CA	D	756	1/1	0.99	0.06	-2.89	22,22,22,22	0
3	CA	A	759	1/1	0.91	0.05	-3.26	15,15,15,15	0
3	CA	B	401	1/1	0.98	0.14	-	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.