Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:03 AM GMT

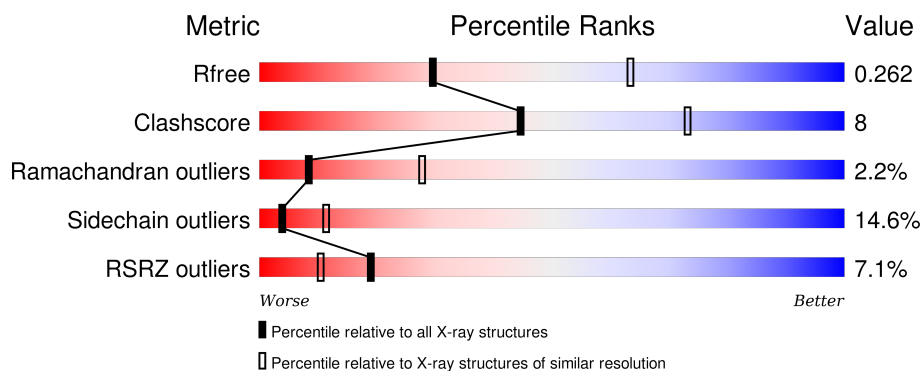|		
PDB ID	:	2FGH
Title	:	ATP bound gelsolin
Authors	:	Ma, Q.; Robinson, R.C.; Burtnick, L.D.; Urosev, D.
Deposited on	:	2005-12-22
Resolution	:	2.80 Å(reported)

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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 2.80 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	Percentile Ranks	Value
Rfree		0.262
Clashscore		8
Ramachandran outliers		2.2%
Sidechain outliers		14.6%
RSRZ outliers		7.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▊ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	731	7% / 74% / 21% / · ··
1	B	731	7% / 72% / 22% / · ··

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11378 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.
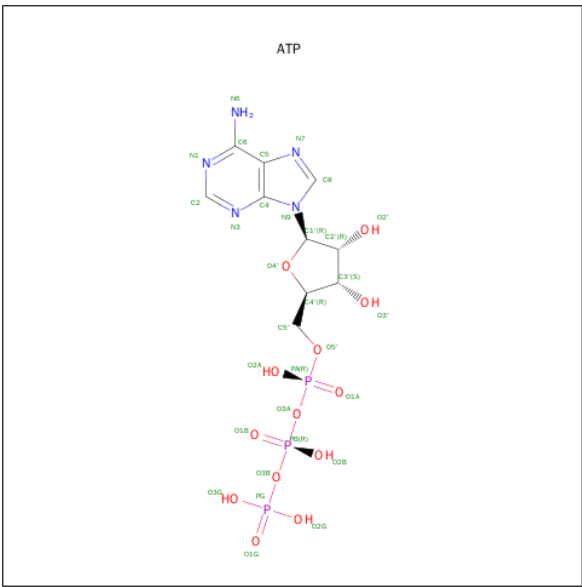
- Molecule 1 is a protein called gelsolin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total 5633	C 3564	N 981	O 1072	S 16	0	0	0
1	B	721	Total 5633	C 3564	N 981	O 1072	S 16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	INSERTION	UNP Q28372
B	25	MET	-	INSERTION	UNP Q28372

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

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

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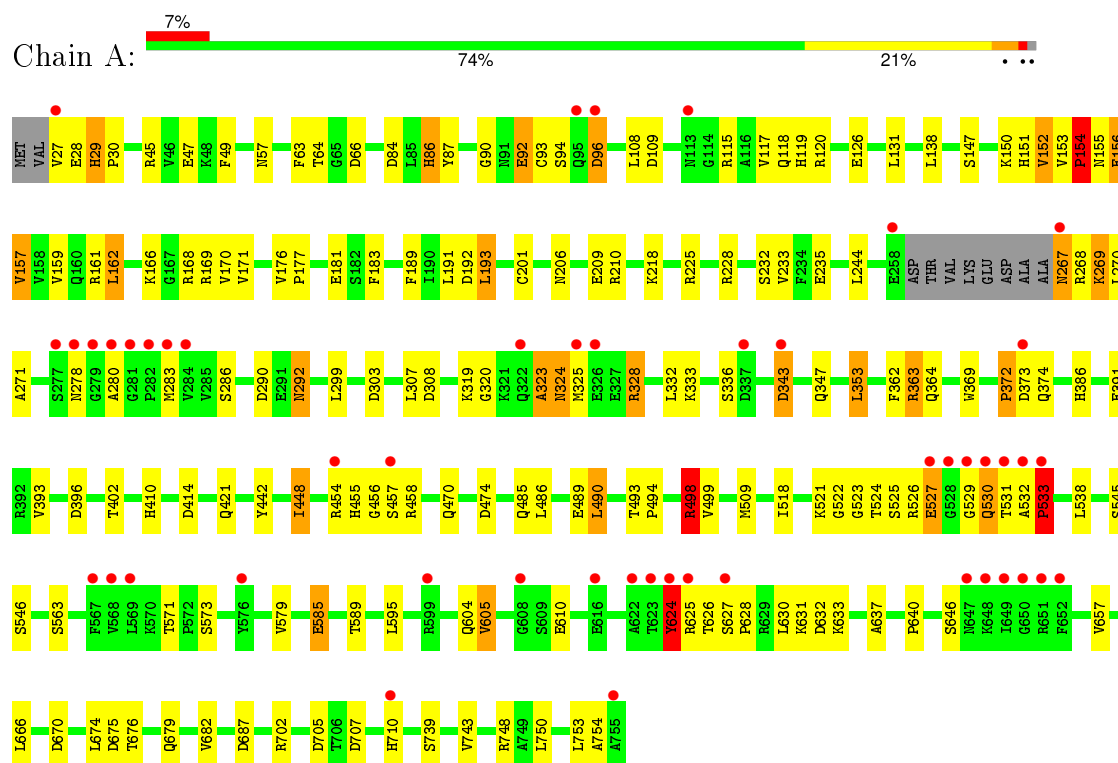| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	31	10	5	13	3	0	0

- Molecule 3 is water.

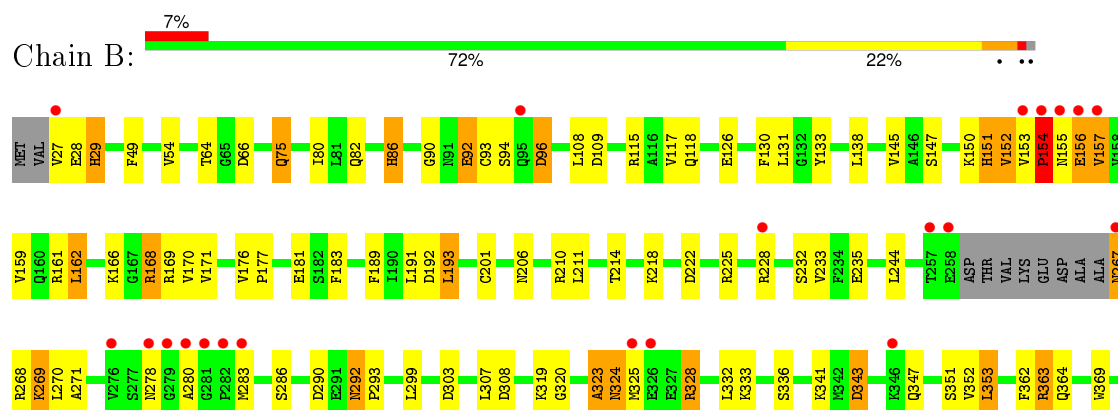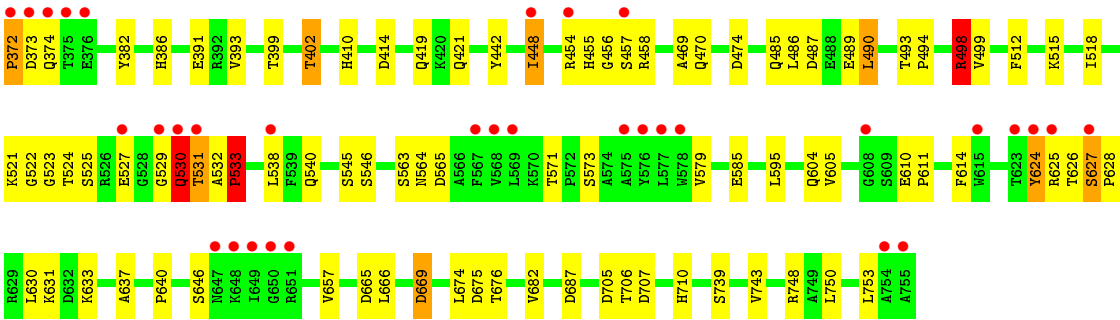| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total 27	O 27	0	0
3	B	23	Total 23	O 23	0	0

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: gelsolin

- Molecule 1: gelsolin

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	167.34Å 167.34Å 149.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-2.80) 98.9 (19.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.49 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.242 , 0.265 0.241 , 0.262	Depositor DCC
R_{free} test set	2650 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.32$	Xtriage
Outliers	0 of 52123 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11378	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.50	0/5766	0.81	15/7812 (0.2%)
1	B	0.51	0/5766	0.81	17/7812 (0.2%)
All	All	0.50	0/11532	0.81	32/15624 (0.2%)

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	414	ASP	CB-CG-OD2	7.35	124.92	118.30
1	B	498	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	474	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	498	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	A	414	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	151	HIS	CB-CA-C	-6.08	98.25	110.40
1	B	474	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	373	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	705	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	670	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	707	ASP	CB-CG-OD2	5.73	123.46	118.30
1	B	343	ASP	CB-CG-OD2	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	487	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	343	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	290	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	96	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	222	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	96	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	373	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	687	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	687	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	707	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	290	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	669	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	303	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	665	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	303	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	396	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	66	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	705	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	308	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	624	TYR	Peptide
1	A	86	HIS	Sidechain
1	B	624	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5633	0	5493	94	1
1	B	5633	0	5493	84	1
2	A	31	0	12	1	0
2	B	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	0	22	0
3	B	23	0	0	9	0
All	All	11378	0	11010	177	1

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 (177) 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:B:152:VAL:O	1:B:153:VAL:HG13	1.66	0.94
1:A:152:VAL:O	1:A:153:VAL:HG13	1.70	0.92
1:B:75:GLN:HG3	3:B:9387:HOH:O	1.69	0.92
1:B:627:SER:HA	3:B:9398:HOH:O	1.72	0.90
1:A:624:TYR:HA	3:A:5397:HOH:O	1.71	0.88
1:B:151:HIS:CE1	3:B:9394:HOH:O	2.28	0.86
1:B:153:VAL:HB	1:B:157:VAL:HG21	1.57	0.85
1:A:86:HIS:CE1	3:A:5381:HOH:O	2.30	0.84
1:A:267:ASN:O	1:A:267:ASN:ND2	2.11	0.84
1:A:153:VAL:HB	1:A:157:VAL:HG21	1.60	0.82
1:B:267:ASN:ND2	1:B:267:ASN:O	2.14	0.81
1:B:154:PRO:O	1:B:157:VAL:HG22	1.83	0.79
1:A:151:HIS:CE1	3:A:5383:HOH:O	2.36	0.77
1:A:154:PRO:O	1:A:157:VAL:HG22	1.85	0.77
1:A:86:HIS:CE1	1:A:119:HIS:HD2	2.03	0.76
1:A:86:HIS:ND1	3:A:5381:HOH:O	2.17	0.75
1:A:151:HIS:ND1	3:A:5383:HOH:O	2.20	0.73
1:B:86:HIS:CE1	1:B:133:TYR:CE2	2.77	0.73
1:A:498:ARG:HH11	1:A:498:ARG:HG2	1.54	0.71
1:A:86:HIS:CG	3:A:5381:HOH:O	2.44	0.70
1:B:86:HIS:CE1	1:B:133:TYR:HE2	2.10	0.70
1:B:86:HIS:CE1	3:B:9402:HOH:O	2.44	0.70
1:B:292:ASN:HD22	1:B:292:ASN:H	1.38	0.69
1:B:498:ARG:HG2	1:B:498:ARG:HH11	1.56	0.69
1:A:117:VAL:HG12	1:A:119:HIS:CE1	2.28	0.69
1:A:63:PHE:CD1	1:A:151:HIS:HE1	2.11	0.68
1:B:86:HIS:ND1	3:B:9402:HOH:O	2.27	0.67
1:A:626:THR:O	1:A:628:PRO:HD3	1.94	0.67
1:A:155:ASN:O	1:A:156:GLU:HB2	1.93	0.67
1:A:485:GLN:O	1:A:489:GLU:HG3	1.93	0.67
1:B:155:ASN:O	1:B:156:GLU:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:THR:HG21	3:A:5401:HOH:O	1.95	0.67
1:B:626:THR:O	1:B:628:PRO:HD3	1.95	0.66
1:A:152:VAL:O	1:A:153:VAL:CG1	2.44	0.66
1:B:152:VAL:O	1:B:153:VAL:CG1	2.41	0.66
1:A:86:HIS:ND1	1:A:119:HIS:HD2	1.94	0.65
1:B:485:GLN:O	1:B:489:GLU:HG3	1.95	0.65
1:A:151:HIS:C	3:A:5391:HOH:O	2.35	0.65
1:A:292:ASN:H	1:A:292:ASN:HD22	1.43	0.65
1:B:86:HIS:CD2	1:B:86:HIS:N	2.66	0.64
1:B:151:HIS:ND1	3:B:9394:HOH:O	2.28	0.63
1:A:84:ASP:HB3	1:A:86:HIS:HE1	1.66	0.60
1:B:675:ASP:OD1	1:B:676:THR:O	2.19	0.60
1:A:86:HIS:CE1	1:A:119:HIS:CD2	2.89	0.60
1:A:209:GLU:HG2	3:A:5398:HOH:O	2.02	0.60
1:A:93:CYS:HA	3:A:5389:HOH:O	2.02	0.60
1:B:353:LEU:HD23	1:B:353:LEU:N	2.15	0.59
1:A:63:PHE:CE1	1:A:151:HIS:CE1	2.91	0.59
1:A:119:HIS:CG	3:A:5390:HOH:O	2.55	0.59
1:B:86:HIS:ND1	1:B:130:PHE:HD1	2.00	0.59
1:A:754:ALA:HB2	3:A:5387:HOH:O	2.02	0.58
1:A:119:HIS:CE1	3:A:5390:HOH:O	2.55	0.58
1:A:702:ARG:HD3	3:A:5400:HOH:O	2.02	0.58
1:A:353:LEU:N	1:A:353:LEU:HD23	2.18	0.57
1:B:27:VAL:O	1:B:28:GLU:HG2	2.04	0.57
1:B:532:ALA:HB1	1:B:533:PRO:HD2	1.86	0.57
1:A:151:HIS:CG	3:A:5383:HOH:O	2.58	0.57
1:A:152:VAL:N	3:A:5391:HOH:O	2.38	0.56
1:B:155:ASN:O	1:B:156:GLU:CB	2.53	0.56
1:A:86:HIS:ND1	1:A:119:HIS:CD2	2.73	0.56
1:A:448:ILE:HD11	1:A:486:LEU:HD22	1.86	0.56
1:A:90:GLY:O	1:A:93:CYS:HB2	2.05	0.56
1:A:155:ASN:O	1:A:156:GLU:CB	2.53	0.55
1:B:448:ILE:HD11	1:B:486:LEU:HD22	1.88	0.55
1:A:63:PHE:HD1	1:A:151:HIS:HE1	1.55	0.55
1:A:57:ASN:HB3	3:A:5395:HOH:O	2.07	0.55
1:A:45:ARG:HD2	1:A:151:HIS:NE2	2.21	0.54
1:A:630:LEU:HD22	2:A:5380:ATP:C8	2.43	0.54
1:A:532:ALA:HB1	1:A:533:PRO:HD2	1.88	0.54
1:B:86:HIS:NE2	1:B:133:TYR:HE2	2.05	0.54
1:A:155:ASN:HB3	3:A:5407:HOH:O	2.08	0.53
1:A:675:ASP:OD1	1:A:676:THR:O	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HG	1:A:193:LEU:HD13	1.91	0.53
1:B:154:PRO:O	1:B:157:VAL:CG2	2.55	0.53
1:A:154:PRO:O	1:A:157:VAL:CG2	2.57	0.52
1:B:270:LEU:HA	1:B:292:ASN:HD21	1.75	0.52
1:B:191:LEU:HG	1:B:193:LEU:HD13	1.91	0.52
1:B:319:LYS:HD2	1:B:328:ARG:HG2	1.92	0.52
1:A:27:VAL:O	1:A:28:GLU:HG2	2.10	0.52
1:A:320:GLY:O	1:A:323:ALA:HB2	2.10	0.52
1:B:117:VAL:HG13	1:B:353:LEU:HD22	1.92	0.51
1:B:630:LEU:HD22	2:B:9380:ATP:C8	2.44	0.51
1:A:109:ASP:CG	1:A:118:GLN:HE21	2.12	0.51
1:B:485:GLN:HB3	3:B:9403:HOH:O	2.10	0.51
1:A:323:ALA:O	1:A:324:ASN:CB	2.57	0.51
1:B:442:TYR:CD2	1:B:525:SER:HB3	2.45	0.51
1:A:57:ASN:CB	3:A:5395:HOH:O	2.57	0.51
1:A:63:PHE:CD1	1:A:151:HIS:CE1	2.95	0.51
1:B:201:CYS:SG	1:B:210:ARG:HG2	2.51	0.51
1:A:442:TYR:CD2	1:A:525:SER:HB3	2.47	0.50
1:B:109:ASP:CG	1:B:118:GLN:HE21	2.15	0.50
1:A:679:GLN:HB3	3:A:5401:HOH:O	2.11	0.49
1:B:54:VAL:HG22	1:B:151:HIS:NE2	2.26	0.49
1:A:269:LYS:HE2	1:A:710:HIS:CE1	2.47	0.49
1:B:323:ALA:O	1:B:324:ASN:CB	2.60	0.49
1:B:442:TYR:HB3	1:B:523:GLY:O	2.12	0.49
1:B:455:HIS:O	1:B:457:SER:N	2.46	0.49
1:B:109:ASP:CB	1:B:118:GLN:HE21	2.25	0.49
1:B:90:GLY:O	1:B:93:CYS:HB2	2.12	0.49
1:B:183:PHE:HA	1:B:189:PHE:CZ	2.48	0.49
1:A:84:ASP:HB3	1:A:86:HIS:CE1	2.47	0.48
1:A:486:LEU:O	1:A:490:LEU:HB2	2.13	0.48
1:A:278:ASN:HB3	1:A:283:MET:HA	1.96	0.48
1:A:270:LEU:HA	1:A:292:ASN:HD21	1.78	0.48
1:B:675:ASP:C	1:B:676:THR:O	2.50	0.48
1:A:181:GLU:OE1	1:B:181:GLU:OE1	2.31	0.48
1:B:278:ASN:HB3	1:B:283:MET:HA	1.95	0.48
1:B:386:HIS:HE1	1:B:640:PRO:O	1.96	0.48
1:A:319:LYS:HD2	1:A:328:ARG:HG2	1.95	0.48
1:B:469:ALA:HB2	3:B:9396:HOH:O	2.14	0.48
1:B:363:ARG:HG2	1:B:369:TRP:CD2	2.49	0.48
1:A:626:THR:O	1:A:628:PRO:CD	2.61	0.47
1:B:64:THR:HG22	1:B:92:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD12	1:A:138:LEU:N	2.30	0.47
1:A:64:THR:HG22	1:A:92:GLU:HG2	1.95	0.47
1:B:118:GLN:O	1:B:351:SER:HA	2.16	0.46
1:A:363:ARG:HG2	1:A:369:TRP:CD2	2.50	0.46
1:A:183:PHE:HA	1:A:189:PHE:CZ	2.50	0.46
1:A:524:THR:CG2	1:A:529:GLY:HA3	2.46	0.46
1:B:293:PRO:HG3	1:B:710:HIS:HB2	1.97	0.46
1:B:540:GLN:NE2	1:B:565:ASP:OD1	2.47	0.46
1:B:630:LEU:HD21	1:B:637:ALA:HB2	1.97	0.46
1:A:154:PRO:O	1:A:155:ASN:C	2.55	0.45
1:B:564:ASN:HD21	1:B:628:PRO:HA	1.81	0.45
1:B:626:THR:O	1:B:628:PRO:CD	2.62	0.45
1:B:161:ARG:HG3	1:B:192:ASP:HB3	1.99	0.45
1:B:138:LEU:N	1:B:138:LEU:HD12	2.31	0.45
1:B:80:ILE:HB	3:B:9391:HOH:O	2.16	0.45
1:A:161:ARG:HG3	1:A:192:ASP:HB3	1.99	0.45
1:A:442:TYR:HB3	1:A:523:GLY:O	2.17	0.45
1:B:153:VAL:HA	1:B:154:PRO:HD2	1.86	0.44
1:B:269:LYS:HB2	1:B:706:THR:O	2.18	0.44
1:A:353:LEU:HD11	1:A:362:PHE:HB2	2.00	0.44
1:B:168:ARG:NH2	1:B:669:ASP:OD1	2.50	0.44
1:B:271:ALA:H	1:B:292:ASN:ND2	2.15	0.43
1:B:352:VAL:C	1:B:353:LEU:HD23	2.38	0.43
1:A:410:HIS:ND1	1:A:545:SER:HB3	2.32	0.43
1:A:386:HIS:HE1	1:A:640:PRO:O	2.01	0.43
1:A:630:LEU:HD21	1:A:637:ALA:HB2	1.99	0.43
1:A:455:HIS:O	1:A:457:SER:N	2.50	0.43
1:B:66:ASP:OD2	1:B:145:VAL:HG23	2.17	0.43
1:A:153:VAL:HA	1:A:154:PRO:HD2	1.87	0.43
1:B:211:LEU:O	1:B:214:THR:HB	2.17	0.43
1:B:176:VAL:HB	1:B:177:PRO:HD2	2.01	0.43
1:B:493:THR:N	1:B:494:PRO:CD	2.82	0.43
1:B:82:GLN:OE1	1:B:382:TYR:HA	2.19	0.43
1:B:320:GLY:O	1:B:323:ALA:HB2	2.19	0.43
1:B:530:GLN:CG	1:B:531:THR:H	2.32	0.43
1:A:271:ALA:H	1:A:292:ASN:ND2	2.16	0.43
1:B:512:PHE:O	1:B:515:LYS:HB2	2.19	0.43
1:B:410:HIS:ND1	1:B:545:SER:HB3	2.34	0.43
1:A:119:HIS:CD2	3:A:5390:HOH:O	2.71	0.42
1:A:526:ARG:O	1:A:527:GLU:O	2.38	0.42
1:A:176:VAL:HB	1:A:177:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:THR:N	1:A:494:PRO:CD	2.82	0.42
1:B:353:LEU:HD11	1:B:362:PHE:HB2	2.02	0.42
1:A:126:GLU:HG2	1:A:131:LEU:HD21	2.02	0.42
1:B:486:LEU:O	1:B:490:LEU:HB2	2.20	0.41
1:B:162:LEU:HD11	1:B:183:PHE:CE2	2.55	0.41
1:A:162:LEU:HD11	1:A:183:PHE:CE2	2.55	0.41
1:A:63:PHE:HE1	1:A:151:HIS:CE1	2.37	0.41
1:B:28:GLU:O	1:B:29:HIS:HB2	2.21	0.41
1:B:524:THR:CG2	1:B:529:GLY:HA3	2.51	0.41
1:B:154:PRO:O	1:B:155:ASN:C	2.58	0.41
1:A:201:CYS:SG	1:A:210:ARG:HG2	2.60	0.41
1:A:45:ARG:HD3	1:A:47:GLU:OE2	2.20	0.41
1:A:509:MET:HE1	3:A:5406:HOH:O	2.20	0.41
1:A:109:ASP:CB	1:A:118:GLN:HE21	2.33	0.41
1:A:585:GLU:O	1:A:589:THR:HG22	2.21	0.41
1:A:448:ILE:HD11	1:A:486:LEU:CD2	2.51	0.41
1:A:524:THR:HG23	1:A:529:GLY:HA3	2.03	0.41
1:A:87:TYR:OH	1:A:120:ARG:HD2	2.21	0.41
1:B:399:THR:O	1:B:402:THR:HG22	2.21	0.41
1:A:29:HIS:ND1	1:A:30:PRO:HD2	2.36	0.40
1:B:86:HIS:NE2	1:B:133:TYR:CE2	2.84	0.40
1:B:611:PRO:O	1:B:614:PHE:HB3	2.21	0.40
1:B:126:GLU:HG2	1:B:131:LEU:HD21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ASP:OD2	1:B:419:GLN:OE1[5_545]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	717/731 (98%)	664 (93%)	37 (5%)	16 (2%)	8	28
1	B	717/731 (98%)	664 (93%)	38 (5%)	15 (2%)	9	29
All	All	1434/1462 (98%)	1328 (93%)	75 (5%)	31 (2%)	8	28

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	280	ALA
1	A	324	ASN
1	A	456	GLY
1	A	527	GLU
1	A	533	PRO
1	B	29	HIS
1	B	156	GLU
1	B	280	ALA
1	B	324	ASN
1	B	456	GLY
1	B	527	GLU
1	B	533	PRO
1	A	156	GLU
1	A	323	ALA
1	A	573	SER
1	B	323	ALA
1	B	573	SER
1	A	627	SER
1	B	530	GLN
1	B	627	SER
1	A	154	PRO
1	A	530	GLN
1	A	531	THR
1	B	154	PRO
1	B	531	THR
1	B	372	PRO
1	A	372	PRO
1	B	522	GLY
1	A	522	GLY
1	A	605	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	591/599 (99%)	506 (86%)	85 (14%)	4	12
1	B	591/599 (99%)	503 (85%)	88 (15%)	4	11
All	All	1182/1198 (99%)	1009 (85%)	173 (15%)	4	11

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

Mol	Chain	Res	Type
1	A	49	PHE
1	A	92	GLU
1	A	94	SER
1	A	96	ASP
1	A	108	LEU
1	A	115	ARG
1	A	147	SER
1	A	150	LYS
1	A	152	VAL
1	A	154	PRO
1	A	157	VAL
1	A	159	VAL
1	A	162	LEU
1	A	166	LYS
1	A	168	ARG
1	A	169	ARG
1	A	170	VAL
1	A	171	VAL
1	A	193	LEU
1	A	206	ASN
1	A	218	LYS
1	A	225	ARG
1	A	228	ARG
1	A	232	SER
1	A	233	VAL
1	A	235	GLU
1	A	244	LEU

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Mol	Chain	Res	Type
1	A	267	ASN
1	A	268	ARG
1	A	269	LYS
1	A	286	SER
1	A	292	ASN
1	A	299	LEU
1	A	307	LEU
1	A	325	MET
1	A	328	ARG
1	A	332	LEU
1	A	333	LYS
1	A	336	SER
1	A	343	ASP
1	A	347	GLN
1	A	353	LEU
1	A	363	ARG
1	A	364	GLN
1	A	372	PRO
1	A	374	GLN
1	A	391	GLU
1	A	393	VAL
1	A	402	THR
1	A	421	GLN
1	A	448	ILE
1	A	454	ARG
1	A	458	ARG
1	A	470	GLN
1	A	490	LEU
1	A	498	ARG
1	A	499	VAL
1	A	518	ILE
1	A	521	LYS
1	A	530	GLN
1	A	533	PRO
1	A	538	LEU
1	A	546	SER
1	A	563	SER
1	A	571	THR
1	A	579	VAL
1	A	585	GLU
1	A	595	LEU
1	A	604	GLN

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Mol	Chain	Res	Type
1	A	605	VAL
1	A	610	GLU
1	A	624	TYR
1	A	625	ARG
1	A	631	LYS
1	A	633	LYS
1	A	646	SER
1	A	657	VAL
1	A	666	LEU
1	A	674	LEU
1	A	682	VAL
1	A	739	SER
1	A	743	VAL
1	A	748	ARG
1	A	750	LEU
1	A	753	LEU
1	B	49	PHE
1	B	75	GLN
1	B	86	HIS
1	B	92	GLU
1	B	94	SER
1	B	96	ASP
1	B	108	LEU
1	B	115	ARG
1	B	147	SER
1	B	150	LYS
1	B	152	VAL
1	B	154	PRO
1	B	157	VAL
1	B	159	VAL
1	B	162	LEU
1	B	166	LYS
1	B	168	ARG
1	B	169	ARG
1	B	170	VAL
1	B	171	VAL
1	B	193	LEU
1	B	206	ASN
1	B	218	LYS
1	B	225	ARG
1	B	228	ARG
1	B	232	SER

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Mol	Chain	Res	Type
1	B	233	VAL
1	B	235	GLU
1	B	244	LEU
1	B	267	ASN
1	B	268	ARG
1	B	269	LYS
1	B	286	SER
1	B	292	ASN
1	B	299	LEU
1	B	307	LEU
1	B	325	MET
1	B	328	ARG
1	B	332	LEU
1	B	333	LYS
1	B	336	SER
1	B	341	LYS
1	B	343	ASP
1	B	347	GLN
1	B	353	LEU
1	B	363	ARG
1	B	364	GLN
1	B	372	PRO
1	B	374	GLN
1	B	391	GLU
1	B	393	VAL
1	B	402	THR
1	B	421	GLN
1	B	448	ILE
1	B	454	ARG
1	B	458	ARG
1	B	470	GLN
1	B	490	LEU
1	B	498	ARG
1	B	499	VAL
1	B	518	ILE
1	B	521	LYS
1	B	530	GLN
1	B	533	PRO
1	B	538	LEU
1	B	546	SER
1	B	563	SER
1	B	571	THR

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Mol	Chain	Res	Type
1	B	579	VAL
1	B	585	GLU
1	B	595	LEU
1	B	604	GLN
1	B	605	VAL
1	B	610	GLU
1	B	624	TYR
1	B	625	ARG
1	B	631	LYS
1	B	633	LYS
1	B	646	SER
1	B	657	VAL
1	B	666	LEU
1	B	674	LEU
1	B	682	VAL
1	B	739	SER
1	B	743	VAL
1	B	748	ARG
1	B	750	LEU
1	B	753	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	118	GLN
1	A	119	HIS
1	A	151	HIS
1	A	164	GLN
1	A	195	ASN
1	A	215	GLN
1	A	230	GLN
1	A	292	ASN
1	A	374	GLN
1	A	386	HIS
1	A	459	GLN
1	A	507	HIS
1	A	564	ASN
1	A	647	ASN
1	A	710	HIS
1	B	91	ASN
1	B	118	GLN

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Mol	Chain	Res	Type
1	B	160	GLN
1	B	164	GLN
1	B	195	ASN
1	B	230	GLN
1	B	292	ASN
1	B	374	GLN
1	B	386	HIS
1	B	459	GLN
1	B	507	HIS
1	B	564	ASN
1	B	647	ASN

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 ⓘ

2 ligands 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	ATP	A	5380	-	24,33,33	0.95	2 (8%)	31,52,52	3.14	8 (25%)
2	ATP	B	9380	-	24,33,33	1.18	3 (12%)	31,52,52	3.06	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
2	ATP	A	5380	-	-	0/18/38/38	0/3/3/3
2	ATP	B	9380	-	-	0/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5380	ATP	C2-N1	2.20	1.38	1.33
2	B	9380	ATP	C2-N1	2.78	1.39	1.33
2	B	9380	ATP	O4'-C1'	2.87	1.44	1.41
2	A	5380	ATP	C2-N3	2.91	1.37	1.32
2	B	9380	ATP	C2-N3	3.27	1.38	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5380	ATP	N3-C2-N1	-10.46	120.88	128.89
2	B	9380	ATP	N3-C2-N1	-9.85	121.35	128.89
2	B	9380	ATP	PA-O3A-PB	-7.94	110.44	132.73
2	A	5380	ATP	PA-O3A-PB	-6.99	113.11	132.73
2	A	5380	ATP	C2'-C1'-N9	-6.42	104.49	114.29
2	B	9380	ATP	C2'-C1'-N9	-6.17	104.86	114.29
2	A	5380	ATP	C1'-N9-C4	-5.19	119.12	126.94
2	B	9380	ATP	C1'-N9-C4	-4.06	120.82	126.94
2	A	5380	ATP	PB-O3B-PG	-3.89	119.62	132.67
2	B	9380	ATP	PB-O3B-PG	-3.82	119.86	132.67
2	B	9380	ATP	O3A-PA-O5'	-3.77	92.94	102.94
2	A	5380	ATP	O3A-PA-O5'	-3.35	94.05	102.94
2	A	5380	ATP	C4'-O4'-C1'	-2.71	106.75	109.72
2	B	9380	ATP	O2B-PB-O3B	2.10	114.61	105.09
2	B	9380	ATP	O4'-C1'-N9	4.66	117.86	108.10
2	A	5380	ATP	O4'-C1'-N9	4.95	118.47	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5380	ATP	1	0
2	B	9380	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(Å²)	Q<0.9
1	A	721/731 (98%)	0.15	49 (6%)	20	12	28, 54, 110, 114	0
1	B	721/731 (98%)	0.23	54 (7%)	17	9	28, 54, 110, 114	0
All	All	1442/1462 (98%)	0.19	103 (7%)	19	10	28, 54, 110, 114	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	ALA	10.8
1	A	531	THR	8.1
1	B	281	GLY	7.5
1	B	27	VAL	7.5
1	A	529	GLY	7.4
1	B	375	THR	7.3
1	A	530	GLN	6.8
1	A	755	ALA	6.6
1	A	528	GLY	6.4
1	B	280	ALA	6.2
1	A	649	ILE	6.0
1	A	281	GLY	5.8
1	B	529	GLY	5.8
1	B	649	ILE	5.5
1	B	374	GLN	5.4
1	B	282	PRO	5.3
1	B	278	ASN	5.2
1	B	755	ALA	4.8
1	B	651	ARG	4.8
1	A	457	SER	4.7
1	B	627	SER	4.6
1	B	608	GLY	4.3
1	B	531	THR	4.2
1	A	278	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	527	GLU	4.0
1	B	530	GLN	4.0
1	B	376	GLU	3.9
1	A	650	GLY	3.9
1	B	373	ASP	3.9
1	B	623	THR	3.9
1	A	533	PRO	3.9
1	A	651	ARG	3.8
1	A	568	VAL	3.8
1	A	648	LYS	3.8
1	B	154	PRO	3.8
1	B	279	GLY	3.7
1	B	527	GLU	3.7
1	B	754	ALA	3.5
1	A	277	SER	3.5
1	A	322	GLN	3.4
1	A	282	PRO	3.4
1	B	155	ASN	3.4
1	B	457	SER	3.4
1	B	625	ARG	3.3
1	A	373	ASP	3.3
1	B	577	LEU	3.2
1	A	343	ASP	3.2
1	B	258	GLU	3.2
1	B	153	VAL	3.2
1	B	326	GLU	3.1
1	B	576	TYR	3.1
1	B	647	ASN	3.1
1	A	624	TYR	3.0
1	A	608	GLY	3.0
1	A	616	GLU	3.0
1	A	625	ARG	3.0
1	A	326	GLU	2.9
1	A	532	ALA	2.9
1	B	568	VAL	2.9
1	A	283	MET	2.9
1	B	257	THR	2.9
1	A	627	SER	2.9
1	A	567	PHE	2.9
1	A	258	GLU	2.8
1	B	648	LYS	2.8
1	B	267	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	599	ARG	2.7
1	A	576	TYR	2.6
1	B	575	ALA	2.6
1	B	538	LEU	2.6
1	B	156	GLU	2.6
1	B	650	GLY	2.5
1	A	623	THR	2.4
1	B	372	PRO	2.4
1	B	448	ILE	2.4
1	B	624	TYR	2.4
1	A	622	ALA	2.4
1	B	567	PHE	2.4
1	B	276	VAL	2.3
1	A	27	VAL	2.3
1	A	454	ARG	2.3
1	A	337	ASP	2.3
1	A	279	GLY	2.3
1	B	95	GLN	2.3
1	B	569	LEU	2.3
1	A	113	ASN	2.3
1	A	652	PHE	2.3
1	A	284	VAL	2.3
1	A	96	ASP	2.2
1	A	647	ASN	2.2
1	A	710	HIS	2.2
1	A	325	MET	2.2
1	B	283	MET	2.2
1	B	346	LYS	2.2
1	B	228	ARG	2.2
1	B	157	VAL	2.2
1	A	95	GLN	2.2
1	A	569	LEU	2.1
1	A	267	ASN	2.1
1	B	578	TRP	2.1
1	B	325	MET	2.1
1	B	454	ARG	2.0
1	B	615	TRP	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
2	ATP	B	9380	31/31	0.96	0.15	-0.94	20,26,33,34	0
2	ATP	A	5380	31/31	0.96	0.15	-1.08	20,26,33,34	0

6.5 Other polymers (i)

There are no such residues in this entry.