



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:54 AM GMT

PDB ID : 3FP2
Title : Crystal structure of Tom71 complexed with Hsp82 C-terminal fragment
Authors : Li, J.; Qian, X.; Hu, J.; Sha, B.
Deposited on : 2009-01-03
Resolution : 1.98 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

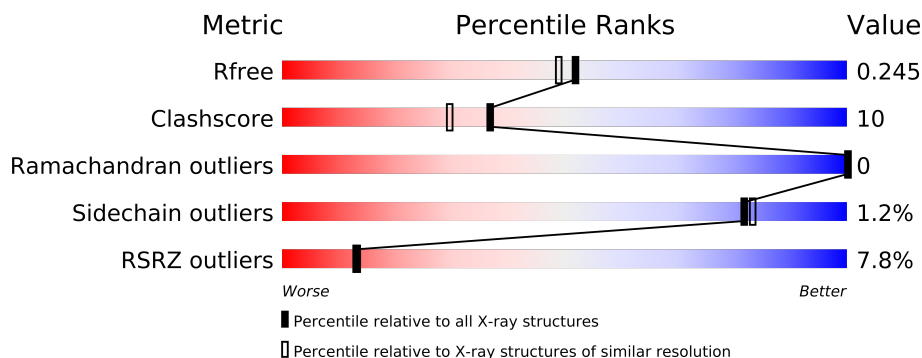
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.98 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}	66092	6577 (2.00-1.96)
Clashscore	79885	8091 (2.00-1.96)
Ramachandran outliers	78287	7989 (2.00-1.96)
Sidechain outliers	78261	7987 (2.00-1.96)
RSRZ outliers	66119	6578 (2.00-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	537	
2	Q	12	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4515 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TPR repeat-containing protein YHR117W.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	22	0
			4037	2578	665	781	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLY	-	EXPRESSION TAG	UNP P38825
A	104	SER	-	EXPRESSION TAG	UNP P38825
A	105	HIS	-	EXPRESSION TAG	UNP P38825
A	106	MET	-	EXPRESSION TAG	UNP P38825

- Molecule 2 is a protein called ATP-dependent molecular chaperone HSP82.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	5	Total	C	N	O	S	0	0	0
			42	24	5	12	1			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

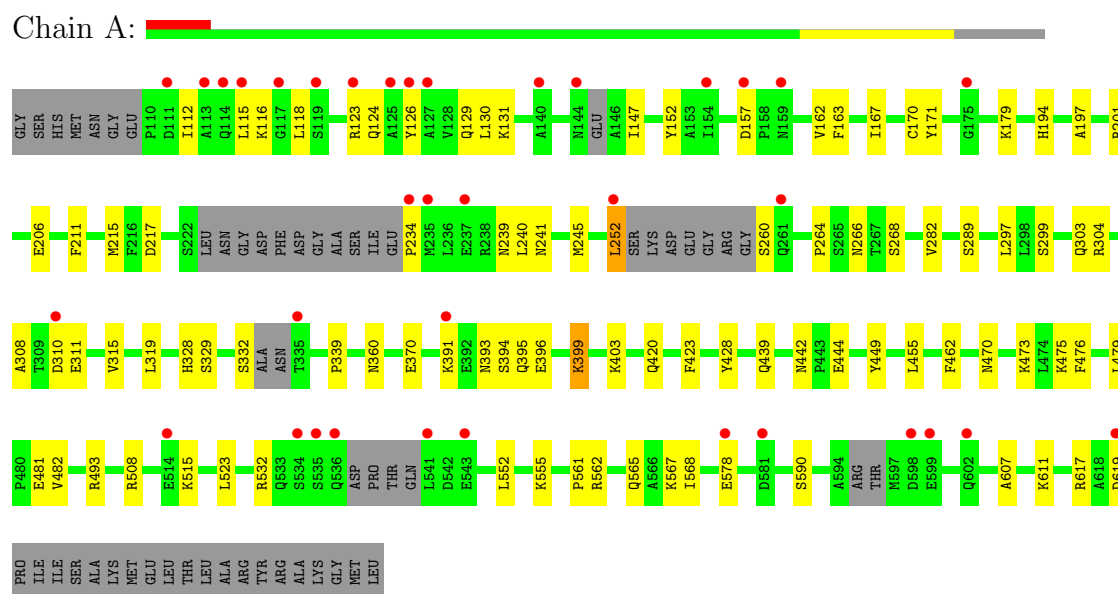
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	430	Total 430	O 430	0	0
5	Q	4	Total 4	O 4	0	0

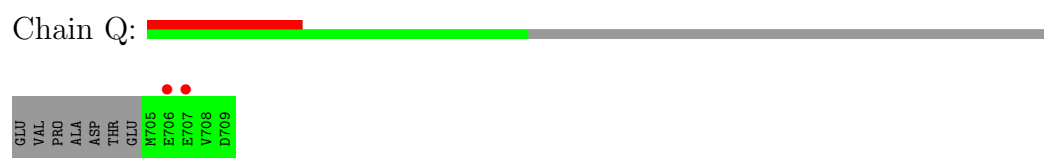
3 Residue-property plots

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: TPR repeat-containing protein YHR117W



- Molecule 2: ATP-dependent molecular chaperone HSP82



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.86Å 116.29Å 150.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.99 – 1.98 7.99 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.8 (7.99-1.98) 96.8 (7.99-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.236 0.210 , 0.245	Depositor DCC
R_{free} test set	2858 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 63.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 56685 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4515	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.82	1/4110 (0.0%)	0.72	1/5544 (0.0%)
2	Q	0.83	0/41	0.64	0/52
All	All	0.82	1/4151 (0.0%)	0.72	1/5596 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	GLU	CB-CG	5.39	1.62	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	GLN	CA-CB-CG	-5.04	102.32	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4037	0	3996	83	0
2	Q	42	0	33	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	430	0	0	21	0
5	Q	4	0	0	0	0
All	All	4515	0	4029	83	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (83) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:420:GLN:HG2	5:A:795:HOH:O	1.65	0.94
1:A:473[A]:LYS:HG3	1:A:482:VAL:HG11	1.55	0.88
1:A:115:LEU:HD22	1:A:126:TYR:CE2	2.14	0.82
1:A:395:GLN:HA	1:A:395:GLN:HE21	1.43	0.82
1:A:442:ASN:HB3	5:A:686:HOH:O	1.80	0.80
1:A:395:GLN:HA	1:A:395:GLN:NE2	2.04	0.72
1:A:439:GLN:HG2	5:A:744:HOH:O	1.90	0.70
1:A:194:HIS:HD2	1:A:197:ALA:H	1.37	0.69
1:A:439:GLN:NE2	1:A:449:TYR:CE1	2.62	0.67
1:A:473[A]:LYS:HG3	1:A:482:VAL:CG1	2.25	0.66
1:A:473[C]:LYS:HG3	1:A:482:VAL:HG11	1.77	0.66
1:A:420:GLN:CG	5:A:795:HOH:O	2.34	0.65
1:A:147[A]:ILE:HD12	1:A:167:ILE:HG23	1.79	0.65
1:A:118:LEU:CD1	1:A:126:TYR:HE2	2.10	0.64
1:A:394:SER:HB2	5:A:737:HOH:O	1.99	0.63
1:A:252:LEU:O	1:A:252:LEU:HD23	1.98	0.63
1:A:439:GLN:NE2	1:A:449:TYR:CD1	2.66	0.63
1:A:532:ARG:NH2	5:A:811:HOH:O	2.32	0.62
1:A:147[A]:ILE:HD11	1:A:170:CYS:HB2	1.82	0.62
1:A:555:LYS:HD3	5:A:652:HOH:O	2.00	0.62
1:A:475[B]:LYS:HE3	5:A:906:HOH:O	2.00	0.62
1:A:328:HIS:HD2	5:A:33:HOH:O	1.82	0.61
1:A:428:TYR:HB3	1:A:455[B]:LEU:HD11	1.84	0.60
1:A:201:ARG:HD3	1:A:217:ASP:OD2	2.02	0.60
1:A:394:SER:HB3	5:A:919:HOH:O	2.00	0.60
1:A:289:SER:HB2	1:A:339:PRO:HB2	1.85	0.59
1:A:201:ARG:CD	1:A:217:ASP:OD2	2.51	0.58
1:A:473[C]:LYS:HG3	1:A:482:VAL:CG1	2.34	0.58
1:A:297:LEU:HD11	1:A:319:LEU:HD22	1.85	0.57
1:A:508:ARG:NH1	5:A:936:HOH:O	2.37	0.57
1:A:565:GLN:HB2	5:A:46:HOH:O	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:396:GLU:O	1:A:399:LYS:HG3	2.05	0.57
1:A:115:LEU:HD22	1:A:126:TYR:CD2	2.39	0.57
1:A:112:ILE:HG22	1:A:116:LYS:HE2	1.86	0.56
1:A:311:GLU:HG3	5:A:880:HOH:O	2.04	0.56
1:A:234:PRO:N	5:A:912:HOH:O	2.39	0.56
1:A:328:HIS:HE1	1:A:370:GLU:OE1	1.89	0.55
1:A:157:ASP:HB3	1:A:163:PHE:HE2	1.72	0.54
1:A:395:GLN:CA	1:A:395:GLN:HE21	2.10	0.54
1:A:394:SER:CB	5:A:737:HOH:O	2.54	0.52
1:A:130:LEU:HD13	1:A:152:TYR:HB3	1.91	0.52
1:A:118:LEU:CD1	1:A:126:TYR:CE2	2.91	0.51
1:A:206:GLU:HB2	1:A:239:ASN:HD21	1.76	0.51
1:A:439:GLN:CG	5:A:744:HOH:O	2.54	0.50
1:A:264:PRO:HB2	1:A:268[B]:SER:OG	2.12	0.49
1:A:475[A]:LYS:HG2	1:A:476:PHE:CE2	2.47	0.49
1:A:299:SER:O	1:A:303[A]:GLN:HG3	2.12	0.48
1:A:211:PHE:O	1:A:215[A]:MET:HG3	2.13	0.48
1:A:473[A]:LYS:NZ	5:A:946:HOH:O	2.47	0.48
1:A:393:ASN:OD1	1:A:395:GLN:HG2	2.14	0.48
1:A:523[B]:LEU:HD22	1:A:552:LEU:CD2	2.44	0.47
1:A:473[A]:LYS:HE2	1:A:482:VAL:HG12	1.96	0.47
1:A:147[A]:ILE:CD1	1:A:167:ILE:HG23	2.44	0.47
1:A:241[B]:ASN:O	1:A:245[B]:MET:HG3	2.15	0.46
1:A:118:LEU:HD11	1:A:126:TYR:HE2	1.81	0.46
1:A:470[A]:ASN:HA	1:A:473[A]:LYS:HD2	1.98	0.46
1:A:403:LYS:HE3	5:A:675:HOH:O	2.15	0.46
1:A:282:VAL:HG11	1:A:303[B]:GLN:HG2	1.99	0.45
1:A:523[B]:LEU:HD22	1:A:552:LEU:HD22	1.99	0.45
1:A:395:GLN:CA	1:A:395:GLN:NE2	2.74	0.45
1:A:428:TYR:CB	1:A:455[B]:LEU:HD11	2.45	0.45
1:A:115:LEU:CD2	1:A:126:TYR:CE2	2.92	0.45
1:A:266:ASN:OD1	1:A:310:ASP:OD1	2.35	0.45
1:A:131:LYS:HD3	1:A:163:PHE:HE1	1.82	0.44
1:A:568:ILE:HD11	1:A:590[A]:SER:OG	2.18	0.44
1:A:116:LYS:HA	1:A:123:ARG:HD2	2.00	0.44
1:A:329[A]:SER:O	1:A:332:SER:HA	2.18	0.43
1:A:473[C]:LYS:HD3	5:A:946:HOH:O	2.17	0.43
1:A:578:GLU:HB3	1:A:617:ARG:HH12	1.83	0.43
1:A:124:GLN:NE2	5:A:726:HOH:O	2.37	0.42
1:A:171:TYR:CD2	1:A:179:LYS:HB3	2.54	0.42
1:A:266:ASN:ND2	1:A:562:ARG:HH22	2.18	0.42
1:A:308:ALA:HB3	1:A:515[A]:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:462:PHE:CD1	1:A:493:ARG:HD2	2.55	0.41
1:A:619:ASP:OD1	1:A:619:ASP:C	2.59	0.41
1:A:201:ARG:HD2	1:A:217:ASP:OD2	2.19	0.41
1:A:304:ARG:HG3	1:A:315:VAL:CG1	2.50	0.41
1:A:470[B]:ASN:OD1	5:A:691:HOH:O	2.22	0.41
1:A:607:ALA:O	1:A:611:LYS:HG3	2.21	0.41
1:A:479:LEU:HB3	1:A:481:GLU:OE1	2.21	0.41
1:A:561:PRO:O	1:A:567[B]:LYS:HE2	2.21	0.41
1:A:215[A]:MET:HE1	1:A:240:LEU:HD13	2.02	0.40
1:A:260:SER:N	1:A:360:ASN:HD21	2.19	0.40

There are no symmetry-related clashes.

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	492/537 (92%)	487 (99%)	5 (1%)	0	100	100
2	Q	3/12 (25%)	3 (100%)	0	0	100	100
All	All	495/549 (90%)	490 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	443/463 (96%)	438 (99%)	5 (1%)	84	85
2	Q	5/11 (46%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	448/474 (94%)	443 (99%)	5 (1%)	82	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	VAL
1	A	252	LEU
1	A	391	LYS
1	A	399	LYS
1	A	423	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	194	HIS
1	A	210	ASN
1	A	239	ASN
1	A	328	HIS
1	A	395	GLN
1	A	417	HIS
1	A	420	GLN
1	A	430	ASN
1	A	547	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	483/537 (89%)	0.33	36 (7%) 14 14	23, 34, 49, 65	0
2	Q	5/12 (41%)	1.44	2 (40%) 1 1	44, 44, 53, 56	0
All	All	488/549 (88%)	0.35	38 (7%) 13 13	23, 35, 49, 65	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	TYR	5.3
1	A	543	GLU	4.8
1	A	252	LEU	4.1
1	A	235	MET	3.7
1	A	111	ASP	3.6
1	A	536	GLN	3.5
1	A	578	GLU	3.5
1	A	113	ALA	3.5
1	A	541	LEU	3.4
1	A	117	GLY	3.3
1	A	125	ALA	3.3
1	A	127	ALA	3.2
1	A	159	ASN	3.1
1	A	599	GLU	2.9
1	A	598	ASP	2.7
1	A	144	ASN	2.7
2	Q	706	GLU	2.7
1	A	140	ALA	2.5
1	A	619	ASP	2.4
1	A	119	SER	2.4
1	A	535	SER	2.4
1	A	237	GLU	2.4
1	A	261	GLN	2.4
1	A	534	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	157	ASP	2.3
1	A	154	ILE	2.3
1	A	115	LEU	2.3
1	A	114	GLN	2.2
1	A	602	GLN	2.2
1	A	310	ASP	2.2
1	A	514	GLU	2.2
1	A	581	ASP	2.2
1	A	234	PRO	2.1
1	A	175	GLY	2.1
1	A	335	THR	2.1
1	A	391	LYS	2.1
1	A	123	ARG	2.1
2	Q	707	GLU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	640	1/1	0.16	1.21	51,51,51,51	0
3	CL	A	1	1/1	0.06	-4.53	68,68,68,68	0

6.5 Other polymers ⓘ

There are no such residues in this entry.