



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:33 PM GMT

PDB ID : 2B9J
Title : Crystal structure of Fus3 with a docking motif from Far1
Authors : Remenyi, A.; Good, M.C.; Bhattacharyya, R.P.; Lim, W.A.
Deposited on : 2005-10-11
Resolution : 2.30 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>

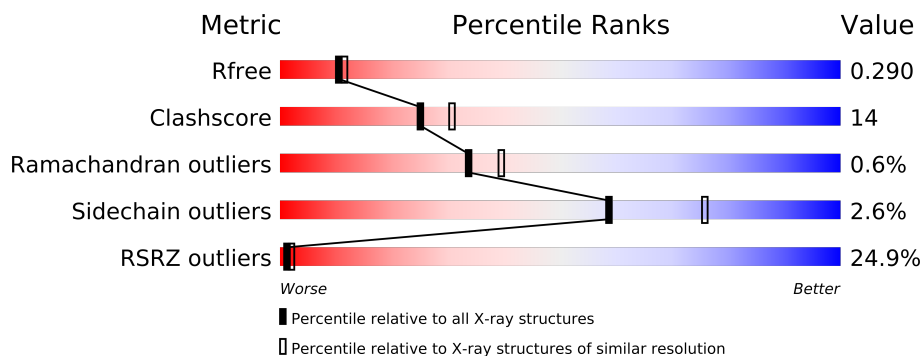
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	353	
2	C	13	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	600	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3093 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 Mitogen-activated protein kinase FUS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2721	1763	460	484	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	VAL	THR	ENGINEERED	UNP P16892
A	182	PHE	TYR	ENGINEERED	UNP P16892

- Molecule 2 is a protein called Cyclin-dependent kinase inhibitor FAR1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			80	52	16	12			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is water.

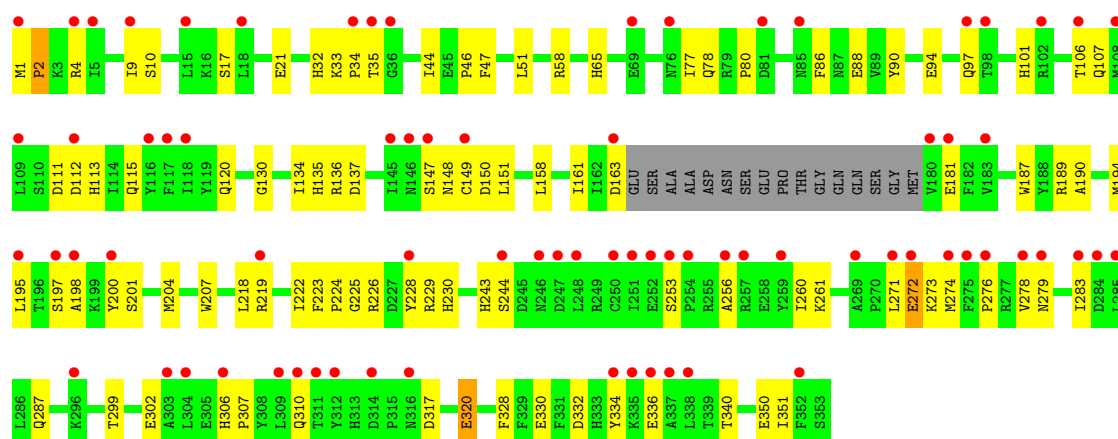
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	255	Total	O	0	0
			255	255		
5	C	9	Total	O	0	0
			9	9		

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: Mitogen-activated protein kinase FUS3

Chain A: 



- Molecule 2: Cyclin-dependent kinase inhibitor FAR1

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.30Å 63.24Å 100.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 42.86 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.30) 96.4 (42.86-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.59 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.263 0.287 , 0.290	Depositor DCC
R_{free} test set	1350 reflections (10.29%)	DCC
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 13125 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3093	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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, ADP

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	0.52	0/2792	0.70	0/3788
2	C	0.47	0/81	0.73	0/109
All	All	0.52	0/2873	0.70	0/3897

There are no bond length outliers.

There are no bond angle outliers.

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	2721	0	2708	74	0
2	C	80	0	85	7	0
3	A	1	0	0	0	0
4	A	27	0	12	0	0
5	A	255	0	0	7	0
5	C	9	0	0	0	0
All	All	3093	0	2805	78	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 14.

All (78) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:134:ILE:HD11	1:A:200:TYR:HB3	1.38	1.05
1:A:10:SER:H	1:A:78:GLN:HE22	1.09	0.95
1:A:1:MET:HG3	1:A:17:SER:HA	1.53	0.89
1:A:134:ILE:CD1	1:A:200:TYR:HB3	2.10	0.82
2:C:73:ARG:HG3	2:C:73:ARG:O	1.80	0.79
1:A:330:GLU:OE2	1:A:334:TYR:HE1	1.65	0.78
1:A:32:HIS:HD2	1:A:35:THR:OG1	1.70	0.75
1:A:189:ARG:HD2	1:A:194:MET:HG2	1.69	0.74
1:A:33:LYS:HB2	1:A:34:PRO:HD3	1.68	0.74
1:A:226:ARG:H	1:A:230:HIS:HD2	1.37	0.72
2:C:80:LEU:HD12	2:C:82:LEU:HD11	1.69	0.72
1:A:271:LEU:HD23	1:A:274:MET:CE	2.21	0.70
1:A:278:VAL:HB	1:A:283:ILE:HD11	1.73	0.69
1:A:271:LEU:HA	1:A:274:MET:HE3	1.75	0.68
2:C:73:ARG:O	2:C:73:ARG:CG	2.40	0.68
1:A:195:LEU:HD13	1:A:260:ILE:HD11	1.76	0.67
1:A:9:ILE:HA	1:A:78:GLN:OE1	1.94	0.67
1:A:330:GLU:OE2	1:A:334:TYR:CE1	2.46	0.66
1:A:10:SER:H	1:A:78:GLN:NE2	1.89	0.65
1:A:226:ARG:H	1:A:230:HIS:CD2	2.13	0.65
1:A:120:GLN:NE2	1:A:151:LEU:H	1.97	0.63
1:A:201:SER:H	1:A:204:MET:HE3	1.62	0.62
1:A:101:HIS:HD2	5:A:764:HOH:O	1.82	0.61
1:A:271:LEU:HD23	1:A:274:MET:HE1	1.84	0.59
1:A:273:LYS:O	1:A:276:PRO:HD3	2.02	0.59
1:A:226:ARG:N	1:A:230:HIS:HD2	2.01	0.57
1:A:4:ARG:HH12	1:A:21:GLU:CD	2.09	0.56
1:A:44:ILE:O	1:A:46:PRO:HD3	2.07	0.54
1:A:107:GLN:O	1:A:219:ARG:NH1	2.40	0.54
1:A:130:GLY:HA3	1:A:320:GLU:O	2.08	0.53
1:A:271:LEU:HD23	1:A:274:MET:HE3	1.90	0.52
1:A:317:ASP:OD2	2:C:73:ARG:NH1	2.43	0.52
1:A:218:LEU:O	1:A:219:ARG:HB2	2.10	0.52
1:A:271:LEU:HD12	1:A:287:GLN:CG	2.41	0.50
1:A:272:GLU:CD	1:A:272:GLU:H	2.15	0.50
1:A:225:GLY:HA2	1:A:230:HIS:CD2	2.47	0.50
1:A:161:ILE:CD1	1:A:328:PHE:HB3	2.44	0.48
1:A:148:ASN:O	1:A:149:CYS:HB2	2.13	0.48
1:A:113:HIS:CD2	2:C:77:PRO:HB2	2.48	0.48
1:A:197:SER:HA	5:A:733:HOH:O	2.14	0.48
1:A:243:HIS:ND1	1:A:244:SER:N	2.61	0.48
1:A:9:ILE:HG22	1:A:78:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:120:GLN:HE22	1:A:151:LEU:H	1.62	0.47
1:A:201:SER:O	1:A:204:MET:HG2	2.15	0.47
1:A:10:SER:N	1:A:78:GLN:HE22	1.92	0.46
1:A:334:TYR:HB3	1:A:336:GLU:O	2.16	0.46
2:C:76:ILE:HG23	2:C:77:PRO:HD2	1.98	0.45
1:A:135:HIS:CE1	1:A:137:ASP:HB3	2.52	0.45
1:A:65:HIS:HE1	5:A:687:HOH:O	1.99	0.45
1:A:307:PRO:O	1:A:310:GLN:HG2	2.17	0.45
1:A:120:GLN:HE22	1:A:150:ASP:HA	1.82	0.44
1:A:80:PRO:HG2	1:A:86:PHE:CD1	2.53	0.44
1:A:106:THR:O	1:A:107:GLN:HG3	2.18	0.44
1:A:299:THR:OG1	1:A:302:GLU:HG3	2.18	0.44
1:A:97:GLN:NE2	1:A:147:SER:H	2.15	0.43
1:A:51:LEU:HD11	1:A:181:GLU:HA	2.00	0.43
1:A:78:GLN:NE2	5:A:635:HOH:O	2.50	0.43
1:A:279:ASN:O	1:A:283:ILE:HD12	2.17	0.43
1:A:77:ILE:HG21	1:A:351:ILE:HG12	2.00	0.43
1:A:187:TRP:CD1	1:A:224:PRO:HA	2.53	0.43
1:A:317:ASP:HB3	2:C:73:ARG:HH12	1.84	0.43
1:A:306:HIS:CG	1:A:307:PRO:HD2	2.54	0.43
1:A:88:GLU:HB2	1:A:90:TYR:CE2	2.54	0.42
1:A:261:LYS:HD3	5:A:846:HOH:O	2.18	0.42
1:A:58:ARG:HD3	1:A:332:ASP:OD2	2.20	0.42
1:A:136:ARG:HD3	1:A:158:LEU:O	2.20	0.41
1:A:111:ASP:OD2	1:A:115:GLN:NE2	2.49	0.41
1:A:253:SER:O	1:A:256:ALA:HB3	2.20	0.41
1:A:222:ILE:HG23	1:A:223:PHE:CD2	2.55	0.41
1:A:271:LEU:HD12	1:A:287:GLN:HG3	2.03	0.41
1:A:340:THR:HG23	5:A:832:HOH:O	2.21	0.41
1:A:1:MET:O	1:A:2:PRO:C	2.59	0.41
1:A:32:HIS:CD2	1:A:35:THR:OG1	2.60	0.41
1:A:46:PRO:HG2	1:A:47:PHE:CE2	2.56	0.41
1:A:306:HIS:HA	1:A:307:PRO:HD3	1.96	0.41
1:A:190:ALA:HA	1:A:207:TRP:CD1	2.56	0.41
1:A:112:ASP:HB2	5:A:672:HOH:O	2.20	0.41
1:A:1:MET:HG2	1:A:2:PRO:HD2	2.04	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	333/353 (94%)	309 (93%)	22 (7%)	2 (1%)	33	39
2	C	9/13 (69%)	7 (78%)	2 (22%)	0	100	100
All	All	342/366 (93%)	316 (92%)	24 (7%)	2 (1%)	33	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ALA
1	A	2	PRO

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	297/319 (93%)	290 (98%)	7 (2%)	61	79
2	C	8/12 (67%)	7 (88%)	1 (12%)	7	7
All	All	305/331 (92%)	297 (97%)	8 (3%)	59	76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	A	163	ASP
1	A	228	TYR
1	A	229	ARG
1	A	272	GLU
1	A	320	GLU
1	A	350	GLU

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Mol	Chain	Res	Type
2	C	73	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	32	HIS
1	A	65	HIS
1	A	85	ASN
1	A	97	GLN
1	A	101	HIS
1	A	120	GLN
1	A	230	HIS
1	A	246	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, 1 is monoatomic - leaving 1 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	ADP	A	500	3	29,29,29	1.02	1 (3%)	45,45,45	1.48	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	500	3	-	0/16/32/32	0/1/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	ADP	PA-O3A	-3.20	1.54	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	ADP	N3-C2-N1	-6.15	123.57	128.71
4	A	500	ADP	C4'-O4'-C1'	3.21	113.24	109.75
4	A	500	ADP	C3'-C2'-C1'	2.70	105.13	100.91
4	A	500	ADP	C4-C5-N7	2.09	111.31	109.52
4	A	500	ADP	C2-N1-C6	2.09	122.55	118.77
4	A	500	ADP	C5-C6-N6	2.09	125.44	120.72

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	337/353 (95%)	1.43	76 (22%) 1 2	10, 21, 47, 61	0
2	C	11/13 (84%)	6.69	11 (100%) 0 0	36, 44, 63, 69	0
All	All	348/366 (95%)	1.59	87 (25%) 1 2	10, 21, 48, 69	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	76	ILE	12.2
2	C	77	PRO	9.3
2	C	82	LEU	8.2
2	C	79	PRO	7.7
2	C	72	LYS	7.3
2	C	73	ARG	6.6
1	A	112	ASP	5.8
1	A	198	ALA	5.6
2	C	75	ASN	5.6
2	C	78	LYS	5.4
2	C	74	GLY	5.3
1	A	312	TYR	5.1
1	A	256	ALA	5.0
1	A	253	SER	4.9
1	A	197	SER	4.5
1	A	274	MET	4.5
1	A	228	TYR	4.5
1	A	275	PHE	4.5
1	A	334	TYR	4.2
1	A	108	MET	4.1
1	A	248	LEU	4.0
1	A	304	LEU	3.9
1	A	18	LEU	3.8
1	A	36	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	146	ASN	3.7
1	A	149	CYS	3.6
1	A	200	TYR	3.6
1	A	246	ASN	3.6
1	A	9	ILE	3.6
1	A	147	SER	3.6
1	A	5	ILE	3.5
2	C	80	LEU	3.5
1	A	285	LEU	3.5
1	A	250	CYS	3.5
1	A	4	ARG	3.4
1	A	145	ILE	3.4
1	A	309	LEU	3.4
1	A	316	ASN	3.3
1	A	336	GLU	3.2
1	A	338	LEU	3.1
1	A	269	ALA	3.0
1	A	116	TYR	3.0
1	A	180	VAL	2.9
1	A	35	THR	2.9
1	A	303	ALA	2.9
1	A	314	ASP	2.9
1	A	310	GLN	2.8
1	A	259	TYR	2.8
1	A	311	THR	2.8
1	A	1	MET	2.7
1	A	252	GLU	2.7
1	A	117	PHE	2.7
1	A	183	VAL	2.7
1	A	98	THR	2.7
1	A	254	PRO	2.6
2	C	81	ASN	2.6
1	A	251	ILE	2.6
1	A	181	GLU	2.6
1	A	97	GLN	2.6
1	A	244	SER	2.6
1	A	69	GLU	2.5
1	A	81	ASP	2.5
1	A	276	PRO	2.5
1	A	15	LEU	2.5
1	A	34	PRO	2.4
1	A	118	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	283	ILE	2.4
1	A	352	PHE	2.3
1	A	85	ASN	2.3
1	A	272	GLU	2.3
1	A	278	VAL	2.3
1	A	284	ASP	2.3
1	A	102	ARG	2.3
1	A	306	HIS	2.3
1	A	163	ASP	2.2
1	A	106	THR	2.2
1	A	247	ASP	2.2
1	A	271	LEU	2.2
1	A	257	ARG	2.2
1	A	279	ASN	2.1
1	A	335	LYS	2.1
1	A	219	ARG	2.1
1	A	76	ASN	2.1
1	A	109	LEU	2.1
1	A	195	LEU	2.1
1	A	337	ALA	2.1
1	A	296	LYS	2.0

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
3	MG	A	600	1/1	0.22	5.09	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ADP	A	500	27/27	0.19	0.02	11,15,18,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.