



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:48 PM GMT

PDB ID : 2J1D
Title : CRYSTALLIZATION OF HDAAM1 C-TERMINAL FRAGMENT
Authors : Lu, J.; Meng, W.; Poy, F.; Eck, M.J.
Deposited on : 2006-08-10
Resolution : 2.25 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>

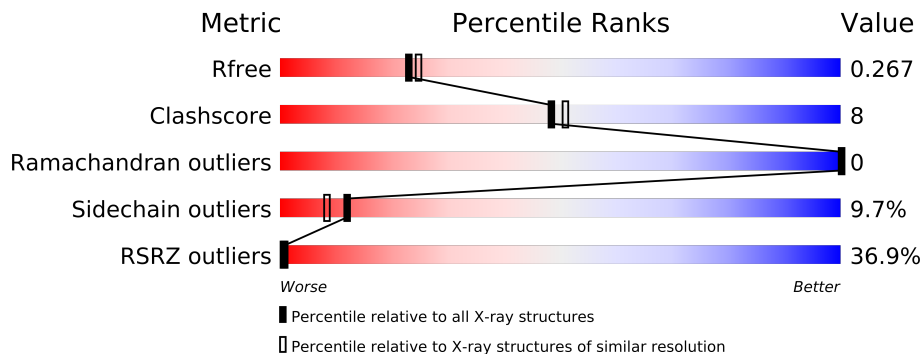
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.25 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	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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	G	483	

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	GOL	G	3027	-	X

2 Entry composition

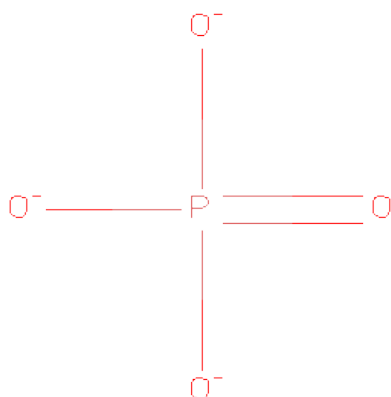
There are 4 unique types of molecules in this entry. The entry contains 3288 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DISHEVELED-ASSOCIATEDACTIVATOR OF MORPHOGENESIS 1.

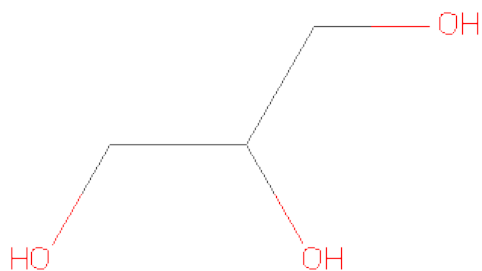
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	396	3202	2024	551	617	10	0	0	1

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	G	1	5	4	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	75	Total	O	0	0
			75	75		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	100.90Å 100.34Å 148.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.25 44.42 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.83-2.25) 98.4 (44.42-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.218 , 0.250 0.262 , 0.267	Depositor DCC
R_{free} test set	1294 reflections (5.57%)	DCC
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.8	EDS
Estimated twinning fraction	0.000 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.000 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.000 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.015 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.000 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 24546 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3288	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.82% 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: GOL, PO4

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	G	0.47	0/3250	0.67	4/4358 (0.1%)

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	G	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	602	SER	N-CA-C	7.99	132.56	111.00
1	G	874	LEU	CA-CB-CG	6.68	130.66	115.30
1	G	602	SER	CB-CA-C	-6.25	98.23	110.10
1	G	759	ARG	NE-CZ-NH2	-5.15	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	830	GLY	Peptide

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	G	3202	0	3225	50	0
2	G	5	0	0	1	0
3	G	6	0	8	0	0
4	G	75	0	0	5	2
All	All	3288	0	3233	50	2

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 8.

All (50) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:752:ASP:OD2	4:G:2025:HOH:O	1.55	1.21
1:G:644:ASP:O	1:G:648:THR:HG23	1.65	0.95
1:G:644:ASP:O	1:G:648:THR:CG2	2.20	0.89
1:G:751:LEU:HA	1:G:754:MET:HE2	1.55	0.88
1:G:894:LYS:O	1:G:898:THR:HG23	1.90	0.71
1:G:923:LYS:HE3	4:G:2068:HOH:O	1.91	0.70
1:G:924:PHE:CE2	1:G:928:VAL:HG21	2.28	0.69
1:G:625:GLY:O	4:G:2005:HOH:O	2.11	0.68
1:G:741:ILE:HD11	4:G:2022:HOH:O	1.94	0.66
1:G:804:VAL:HG13	1:G:960:PHE:HE2	1.62	0.65
1:G:804:VAL:HG13	1:G:960:PHE:CE2	2.33	0.63
1:G:687:VAL:CG1	1:G:743:LEU:HD21	2.30	0.61
1:G:797:ILE:HD11	1:G:887:VAL:HG11	1.81	0.61
1:G:687:VAL:HG11	1:G:743:LEU:HD11	1.84	0.60
1:G:910:LEU:HD22	1:G:928:VAL:HG12	1.84	0.59
1:G:829:ARG:NE	1:G:829:ARG:HA	2.17	0.58
1:G:828:GLN:O	1:G:829:ARG:HB2	2.04	0.57
1:G:924:PHE:CZ	1:G:928:VAL:HG21	2.40	0.57
1:G:798:ARG:NH2	1:G:802:GLU:OE2	2.39	0.55
1:G:644:ASP:O	1:G:648:THR:HG22	2.06	0.55
1:G:957:VAL:HG13	1:G:962:GLU:HB2	1.88	0.55
1:G:602:SER:O	1:G:602:SER:OG	2.15	0.54
1:G:687:VAL:HG12	1:G:743:LEU:HD21	1.88	0.54
1:G:864:VAL:HG22	1:G:868:TYR:HB2	1.91	0.52
1:G:699:LEU:HD13	1:G:730:GLN:HB3	1.93	0.50
1:G:754:MET:HE3	1:G:759:ARG:HA	1.93	0.50
1:G:902:GLY:O	1:G:906:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:743:LEU:O	1:G:746:GLU:HB2	2.11	0.49
1:G:636:VAL:HG12	1:G:640:LEU:HD22	1.93	0.49
1:G:843:ILE:HG23	1:G:856:LEU:HD13	1.95	0.48
1:G:751:LEU:CA	1:G:754:MET:HE2	2.33	0.47
1:G:858:HIS:ND1	1:G:990:ASN:ND2	2.63	0.47
1:G:910:LEU:HD13	1:G:928:VAL:HB	1.96	0.46
1:G:751:LEU:HD22	1:G:754:MET:CE	2.45	0.46
1:G:687:VAL:HG11	1:G:743:LEU:CD1	2.46	0.46
1:G:782:LYS:NZ	2:G:3026:PO4:O1	2.33	0.46
1:G:848:SER:HB3	1:G:851:ASP:O	2.16	0.46
1:G:683:LYS:NZ	1:G:753:ARG:HH22	2.14	0.45
1:G:683:LYS:NZ	1:G:753:ARG:NH2	2.64	0.45
1:G:683:LYS:HZ1	1:G:753:ARG:HH22	1.65	0.45
1:G:636:VAL:HG13	1:G:640:LEU:HD13	2.00	0.44
1:G:906:VAL:HG12	1:G:932:ILE:HD11	2.00	0.43
1:G:687:VAL:CG1	1:G:743:LEU:HD11	2.47	0.43
1:G:623:LEU:O	1:G:624:GLU:HB3	2.19	0.43
1:G:603:ILE:HD12	1:G:604:PRO:O	2.18	0.43
1:G:925:VAL:HG23	4:G:2067:HOH:O	2.20	0.42
1:G:828:GLN:OE1	1:G:829:ARG:N	2.43	0.41
1:G:751:LEU:HD22	1:G:754:MET:HE1	2.03	0.40
1:G:855:THR:H	1:G:858:HIS:CD2	2.39	0.40
1:G:858:HIS:HB3	1:G:990:ASN:HD21	1.86	0.40

All (2) 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	Distance(Å)	Clash(Å)
4:G:2054:HOH:O	4:G:2068:HOH:O[6_555]	1.65	0.55
4:G:2030:HOH:O	4:G:2055:HOH:O[6_554]	1.75	0.45

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	G	392/483 (81%)	383 (98%)	9 (2%)	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	G	352/438 (80%)	318 (90%)	34 (10%)	12	8

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	610	LEU
1	G	615	TRP
1	G	624	GLU
1	G	627	VAL
1	G	635	LYS
1	G	645	LEU
1	G	648	THR
1	G	683	LYS
1	G	685	LEU
1	G	686	SER
1	G	703	LEU
1	G	741	ILE
1	G	745	GLU
1	G	759	ARG
1	G	772	GLN
1	G	790	VAL
1	G	795	GLU
1	G	798	ARG
1	G	804	VAL
1	G	806	ARG
1	G	828	GLN
1	G	856	LEU
1	G	857	LEU
1	G	860	LEU
1	G	863	ILE

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Mol	Chain	Res	Type
1	G	874	LEU
1	G	892	LEU
1	G	898	THR
1	G	899	LEU
1	G	930	GLN
1	G	934	VAL
1	G	951	ASP
1	G	970	ASP
1	G	1001	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	697	ASN
1	G	883	GLN
1	G	888	ASN
1	G	919	GLN
1	G	990	ASN
1	G	992	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 ⓘ

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	PO4	G	3026	-	4,4,4	0.24	0	6,6,6	0.33	0
3	GOL	G	3027	-	5,5,5	0.35	0	5,5,5	0.72	0

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	PO4	G	3026	-	-	0/0/0/0	0/0/0/0
3	GOL	G	3027	-	-	0/4/4/4	0/0/0/0

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	G	396/483 (81%)	1.91	147 (37%) 1 0	48, 65, 103, 106	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1008	ALA	11.5
1	G	1023	ALA	8.6
1	G	1010	LEU	8.6
1	G	1016	ARG	8.1
1	G	1004	ALA	7.9
1	G	1011	LYS	7.7
1	G	1025	GLU	7.3
1	G	1020	MET	6.9
1	G	1014	ARG	6.3
1	G	1002	ARG	6.2
1	G	1006	MET	6.2
1	G	1007	GLU	5.7
1	G	1001	GLU	5.7
1	G	1022	LYS	5.6
1	G	1018	ARG	5.4
1	G	1013	GLN	5.4
1	G	1009	GLN	5.4
1	G	937	PHE	5.3
1	G	1019	LYS	5.3
1	G	1005	ARG	5.1
1	G	1012	GLU	5.0
1	G	994	ARG	5.0
1	G	1017	GLU	4.9
1	G	995	LYS	4.6
1	G	1021	ARG	4.5
1	G	1003	ARG	4.4
1	G	624	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	1015	GLU	4.2
1	G	933	THR	4.2
1	G	997	LYS	4.0
1	G	894	LYS	3.9
1	G	993	MET	3.9
1	G	621	ASN	3.6
1	G	965	GLY	3.6
1	G	892	LEU	3.5
1	G	1024	LYS	3.5
1	G	816	VAL	3.4
1	G	613	PHE	3.4
1	G	833	TYR	3.4
1	G	860	LEU	3.3
1	G	903	LEU	3.2
1	G	647	ARG	3.2
1	G	817	VAL	3.2
1	G	794	VAL	3.2
1	G	983	VAL	3.1
1	G	734	PHE	3.1
1	G	826	LYS	3.1
1	G	998	GLU	3.1
1	G	813	LEU	3.0
1	G	704	LYS	3.0
1	G	623	LEU	3.0
1	G	939	PHE	3.0
1	G	618	LEU	3.0
1	G	966	LYS	3.0
1	G	928	VAL	2.9
1	G	912	TYR	2.9
1	G	601	LYS	2.9
1	G	652	TYR	2.9
1	G	764	MET	2.9
1	G	890	THR	2.9
1	G	610	LEU	2.8
1	G	735	VAL	2.8
1	G	642	LEU	2.8
1	G	645	LEU	2.8
1	G	952	LEU	2.8
1	G	963	GLU	2.8
1	G	914	LYS	2.8
1	G	741	ILE	2.8
1	G	640	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	698	ILE	2.7
1	G	829	ARG	2.7
1	G	622	LYS	2.7
1	G	723	LEU	2.6
1	G	731	LEU	2.6
1	G	783	PHE	2.6
1	G	911	GLU	2.6
1	G	932	ILE	2.6
1	G	869	PRO	2.6
1	G	921	GLY	2.6
1	G	996	LYS	2.5
1	G	820	PHE	2.5
1	G	738	LYS	2.5
1	G	840	LEU	2.5
1	G	964	ALA	2.5
1	G	760	PHE	2.5
1	G	753	ARG	2.5
1	G	864	VAL	2.5
1	G	946	LEU	2.5
1	G	713	ALA	2.5
1	G	831	ASN	2.5
1	G	931	PHE	2.5
1	G	615	TRP	2.5
1	G	757	ALA	2.5
1	G	714	ILE	2.5
1	G	761	LEU	2.4
1	G	797	ILE	2.4
1	G	866	ASN	2.4
1	G	830	GLY	2.4
1	G	958	LYS	2.4
1	G	870	SER	2.4
1	G	924	PHE	2.4
1	G	856	LEU	2.3
1	G	887	VAL	2.3
1	G	925	VAL	2.3
1	G	942	VAL	2.3
1	G	805	PHE	2.3
1	G	861	ILE	2.3
1	G	729	GLU	2.3
1	G	699	LEU	2.3
1	G	777	LEU	2.3
1	G	693	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	754	MET	2.3
1	G	638	LYS	2.3
1	G	970	ASP	2.3
1	G	823	TYR	2.2
1	G	843	ILE	2.2
1	G	907	GLU	2.2
1	G	710	ILE	2.2
1	G	818	LEU	2.2
1	G	837	ILE	2.2
1	G	809	ALA	2.2
1	G	694	GLN	2.2
1	G	850	ILE	2.2
1	G	900	ARG	2.2
1	G	607	THR	2.2
1	G	1000	GLU	2.1
1	G	609	ALA	2.1
1	G	728	LEU	2.1
1	G	874	LEU	2.1
1	G	868	TYR	2.1
1	G	919	GLN	2.1
1	G	992	ASN	2.1
1	G	889	MET	2.1
1	G	603	ILE	2.1
1	G	955	LYS	2.1
1	G	687	VAL	2.1
1	G	863	ILE	2.1
1	G	649	PHE	2.1
1	G	751	LEU	2.1
1	G	824	MET	2.1
1	G	834	GLY	2.1
1	G	865	GLU	2.1
1	G	604	PRO	2.0
1	G	929	SER	2.0
1	G	702	ARG	2.0
1	G	804	VAL	2.0
1	G	811	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	GOL	G	3027	6/6	0.41	3.56	99,100,100,100	0
2	PO4	G	3026	5/5	0.10	-11.86	72,72,74,75	0

6.5 Other polymers

There are no such residues in this entry.