



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:03 PM UTC

PDB ID : 2J1D / pdb_00002j1d
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

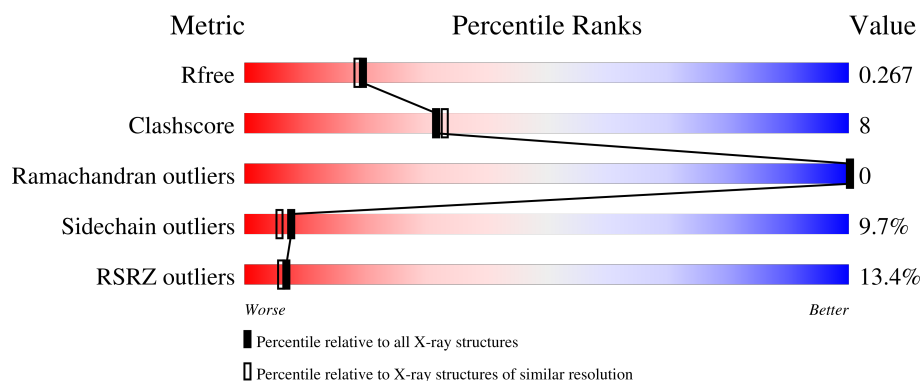
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	G	483	

2 Entry composition [i](#)

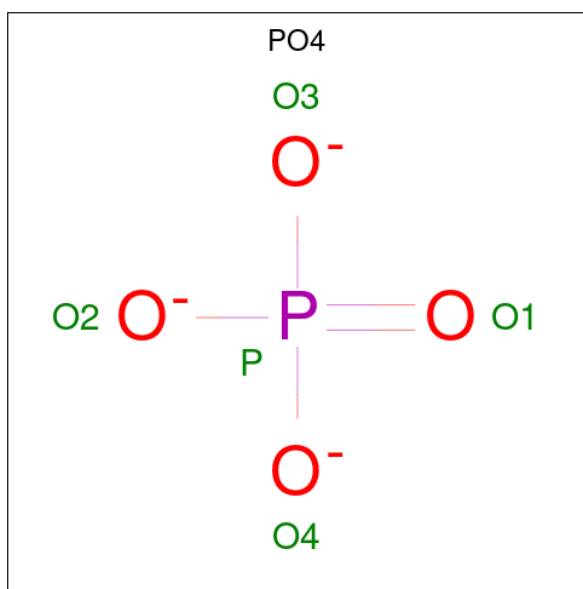
There are 4 unique types of molecules in this entry. The entry contains 3288 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DISHEVELED-ASSOCIATED ACTIVATOR 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 (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

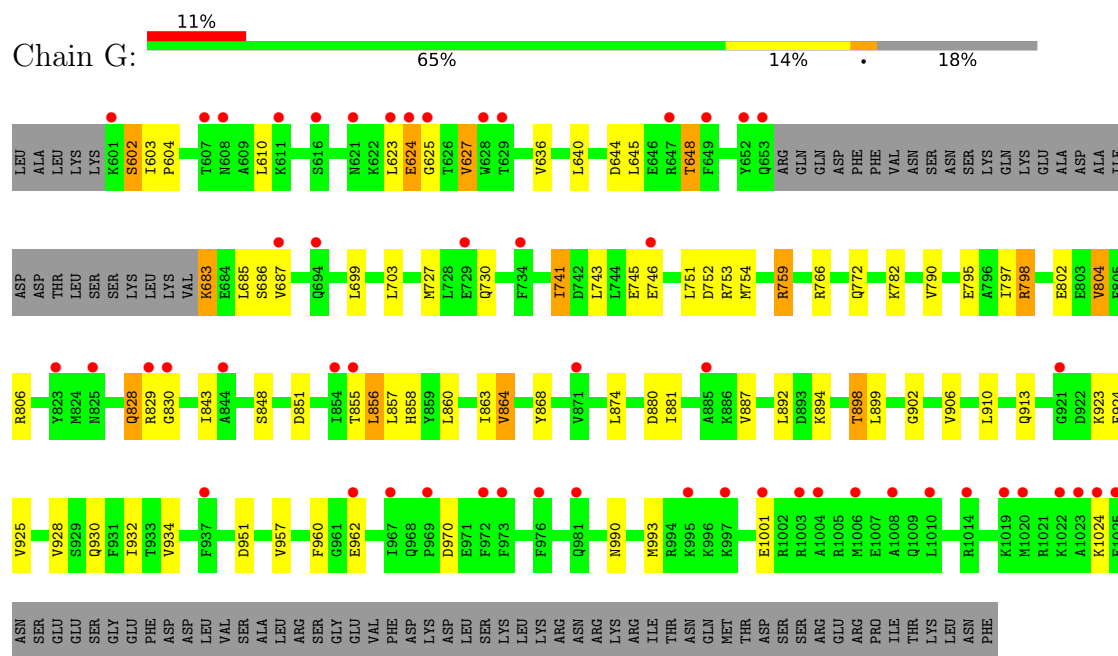
- Molecule 4 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: DISHEVELED-ASSOCIATED ACTIVATOR OF MORPHOGENESIS 1



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 19.83 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.83-2.25) 98.2 (19.83-2.55)	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 (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
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
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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.63	2/3250 (0.1%)	0.93	7/4358 (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	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1024	LYS	C-N	-7.02	1.23	1.33
1	G	881	ILE	CA-CB	6.58	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	602	SER	N-CA-C	9.44	132.56	113.31
1	G	766	ARG	N-CA-C	6.98	121.05	112.54
1	G	602	SER	CB-CA-C	-5.75	98.23	110.76
1	G	602	SER	O-C-N	-5.66	114.84	121.97
1	G	627	VAL	CB-CA-C	-5.64	103.81	112.05
1	G	880	ASP	CA-C-N	5.14	123.48	120.24
1	G	880	ASP	C-N-CA	5.14	123.48	120.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	830	GLY	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	G	3202	0	3225	52	0
2	G	5	0	0	1	0
3	G	6	0	8	1	0
4	G	75	0	0	5	1
All	All	3288	0	3233	52	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 (52) 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: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	0.89
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:993:MET:HE2	3:G:3027:GOL:H2	1.80	0.64
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:602:SER:O	1:G:602:SER:OG	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:754:MET:HE3	1:G:759:ARG:HA	1.86	0.57
1:G:924:PHE:CZ	1:G:928:VAL:HG21	2.40	0.57
1:G:683:LYS:HZ1	1:G:753:ARG:HH22	1.52	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:727:MET:HA	1:G:727:MET:HE2	1.89	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:902:GLY:O	1:G:906:VAL:HG23	2.12	0.50
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:HD22	1:G:754:MET:HE1	1.95	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:CA	1:G:754:MET:HE2	2.33	0.46
1:G:687:VAL:HG11	1:G:743:LEU:CD1	2.46	0.46
1:G:751:LEU:HD22	1:G:754:MET:CE	2.45	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:NH2	2.64	0.45
1:G:683:LYS:NZ	1:G:753:ARG:HH22	2.14	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:623:LEU:O	1:G:624:GLU:HB3	2.19	0.43
1:G:687:VAL:CG1	1:G:743:LEU:HD11	2.47	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: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 (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)
4:G:2054:HOH:O	4:G:2068:HOH:O[6_555]	1.65	0.55

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	G	392/483 (81%)	383 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	G	352/438 (80%)	318 (90%)	34 (10%)	8	6

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

Mol	Chain	Res	Type
1	G	610	LEU
1	G	624	GLU
1	G	627	VAL
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

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Mol	Chain	Res	Type
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
1	G	864	VAL
1	G	874	LEU
1	G	892	LEU
1	G	898	THR
1	G	899	LEU
1	G	913	GLN
1	G	930	GLN
1	G	934	VAL
1	G	951	ASP
1	G	970	ASP
1	G	1001	GLU

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

Mol	Chain	Res	Type
1	G	697	ASN
1	G	775	GLN
1	G	812	GLN
1	G	875	ASN
1	G	883	GLN
1	G	888	ASN
1	G	959	HIS
1	G	990	ASN
1	G	992	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 oligosaccharides 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	0.89	0	6,6,6	0.82	0
3	GOL	G	3027	-	5,5,5	0.43	0	5,5,5	0.65	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
3	GOL	G	3027	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	3027	GOL	O1-C1-C2-C3
3	G	3027	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3026	PO4	1	0
3	G	3027	GOL	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

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%)	1.09	53 (13%) 7 6	48, 65, 103, 106	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1025	GLU	5.3
1	G	1008	ALA	4.3
1	G	1010	LEU	4.3
1	G	1024	LYS	4.2
1	G	1004	ALA	4.1
1	G	830	GLY	4.1
1	G	624	GLU	3.9
1	G	1023	ALA	3.8
1	G	972	PHE	3.5
1	G	962	GLU	3.3
1	G	652	TYR	3.3
1	G	885	ALA	3.2
1	G	601	LYS	3.1
1	G	976	PHE	3.1
1	G	653	GLN	3.0
1	G	937	PHE	3.0
1	G	823	TYR	2.9
1	G	967	ILE	2.8
1	G	623	LEU	2.8
1	G	649	PHE	2.8
1	G	829	ARG	2.8
1	G	746	GLU	2.7
1	G	1020	MET	2.7
1	G	687	VAL	2.6
1	G	607	THR	2.5
1	G	969	PRO	2.5
1	G	625	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	616	SER	2.5
1	G	729	GLU	2.5
1	G	844	ALA	2.5
1	G	1019	LYS	2.4
1	G	694	GLN	2.3
1	G	1022	LYS	2.3
1	G	825	ASN	2.3
1	G	629	THR	2.3
1	G	1001	GLU	2.3
1	G	997	LYS	2.3
1	G	611	LYS	2.2
1	G	628	TRP	2.2
1	G	854	ILE	2.2
1	G	871	VAL	2.2
1	G	973	PHE	2.2
1	G	1014	ARG	2.2
1	G	621	ASN	2.2
1	G	995	LYS	2.2
1	G	647	ARG	2.1
1	G	981	GLN	2.1
1	G	608	ASN	2.1
1	G	734	PHE	2.1
1	G	1006	MET	2.1
1	G	921	GLY	2.1
1	G	1003	ARG	2.0
1	G	855	THR	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	G	3027	6/6	0.83	0.22	99,100,100,100	0
2	PO4	G	3026	5/5	0.94	0.24	72,72,74,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.