



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 01:40 pm BST

PDB ID : 4GV7  
Title : Human ARTD1 (PARP1) - Catalytic domain in complex with inhibitor ME0328  
Authors : Karlberg, T.; Thorsell, A.G.; Lindgren, A.E.G.; Ekblad, T.; Spjut, S.; Andersson, C.D.; Weigelt, J.; Linusson, A.; Elofsson, M.; Schuler, H.  
Deposited on : 2012-08-30  
Resolution : 2.89 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

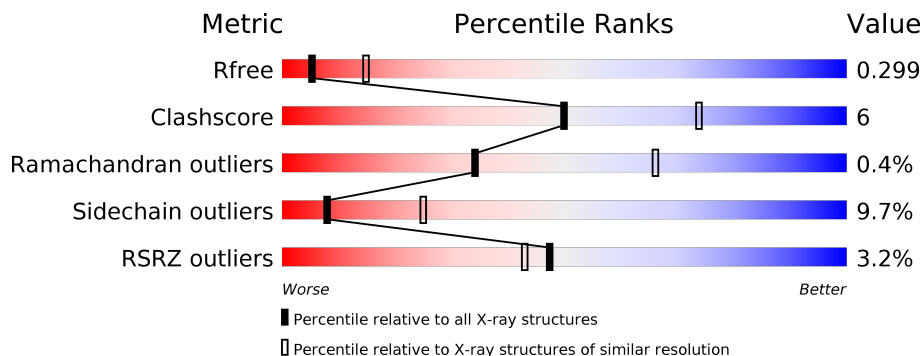
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	A	358	 % 75% 21% ..
1	B	358	 3% 78% 18% ..
1	C	358	 4% 71% 24% ..
1	D	358	 5% 75% 21% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MEW	D	1101	-	X	-	-

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 10988 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 Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	348	2735	1740	462	522	11	0	0	0
1	B	348	2735	1740	462	522	11	0	0	0
1	C	348	2735	1740	462	522	11	0	0	0
1	D	348	2735	1740	462	522	11	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

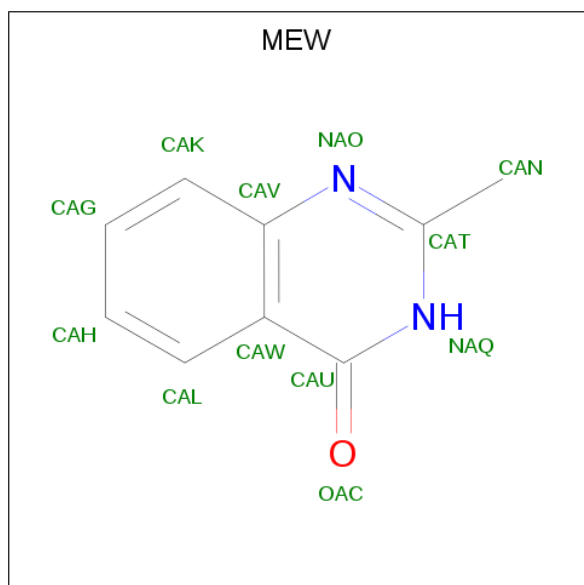
Chain	Residue	Modelled	Actual	Comment	Reference
A	661	MET	-	EXPRESSION TAG	UNP P09874
A	762	ALA	VAL	SEE REMARK 999	UNP P09874
A	1012	ALA	-	EXPRESSION TAG	UNP P09874
A	1013	HIS	-	EXPRESSION TAG	UNP P09874
A	1014	HIS	-	EXPRESSION TAG	UNP P09874
A	1015	HIS	-	EXPRESSION TAG	UNP P09874
A	1016	HIS	-	EXPRESSION TAG	UNP P09874
A	1017	HIS	-	EXPRESSION TAG	UNP P09874
A	1018	HIS	-	EXPRESSION TAG	UNP P09874
B	661	MET	-	EXPRESSION TAG	UNP P09874
B	762	ALA	VAL	SEE REMARK 999	UNP P09874
B	1012	ALA	-	EXPRESSION TAG	UNP P09874
B	1013	HIS	-	EXPRESSION TAG	UNP P09874
B	1014	HIS	-	EXPRESSION TAG	UNP P09874
B	1015	HIS	-	EXPRESSION TAG	UNP P09874
B	1016	HIS	-	EXPRESSION TAG	UNP P09874
B	1017	HIS	-	EXPRESSION TAG	UNP P09874
B	1018	HIS	-	EXPRESSION TAG	UNP P09874
C	661	MET	-	EXPRESSION TAG	UNP P09874
C	762	ALA	VAL	SEE REMARK 999	UNP P09874
C	1012	ALA	-	EXPRESSION TAG	UNP P09874

*Continued on next page...*

Continued from previous page...

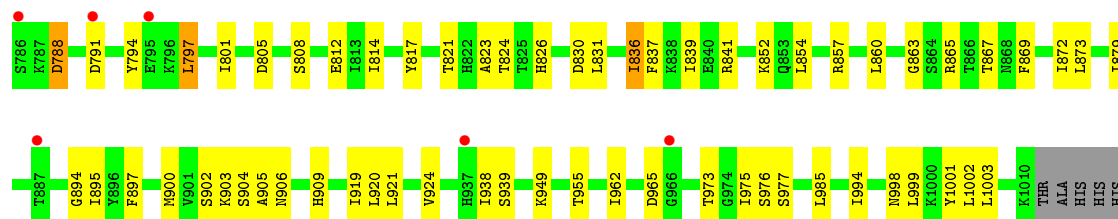
Chain	Residue	Modelled	Actual	Comment	Reference
C	1013	HIS	-	EXPRESSION TAG	UNP P09874
C	1014	HIS	-	EXPRESSION TAG	UNP P09874
C	1015	HIS	-	EXPRESSION TAG	UNP P09874
C	1016	HIS	-	EXPRESSION TAG	UNP P09874
C	1017	HIS	-	EXPRESSION TAG	UNP P09874
C	1018	HIS	-	EXPRESSION TAG	UNP P09874
D	661	MET	-	EXPRESSION TAG	UNP P09874
D	762	ALA	VAL	SEE REMARK 999	UNP P09874
D	1012	ALA	-	EXPRESSION TAG	UNP P09874
D	1013	HIS	-	EXPRESSION TAG	UNP P09874
D	1014	HIS	-	EXPRESSION TAG	UNP P09874
D	1015	HIS	-	EXPRESSION TAG	UNP P09874
D	1016	HIS	-	EXPRESSION TAG	UNP P09874
D	1017	HIS	-	EXPRESSION TAG	UNP P09874
D	1018	HIS	-	EXPRESSION TAG	UNP P09874

- Molecule 2 is 2-methylquinazolin-4(3H)-one (three-letter code: MEW) (formula: C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O).



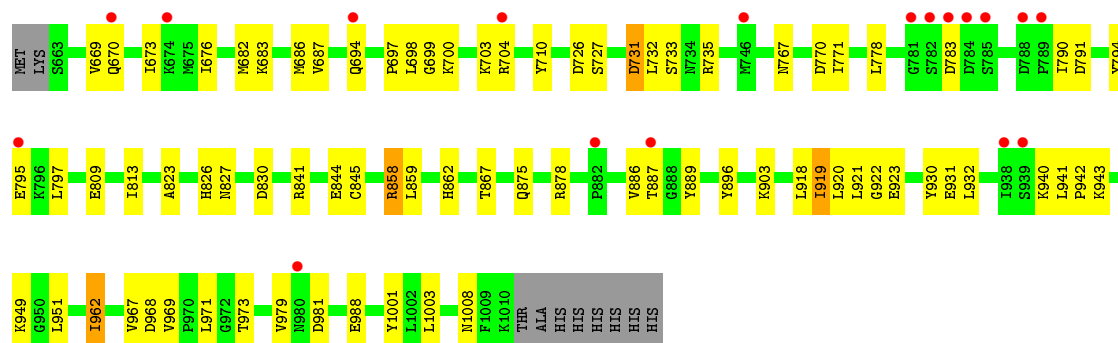
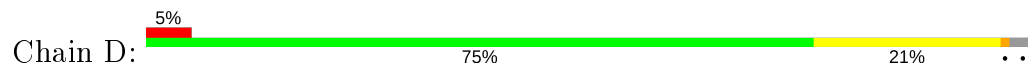
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			12	9	2	1		
2	B	1	Total	C	N	O	0	0
			12	9	2	1		
2	C	1	Total	C	N	O	0	0
			12	9	2	1		
2	D	1	Total	C	N	O	0	0
			12	9	2	1		





HIS  
HIS  
HIS

● Molecule 1: Poly [ADP-ribose] polymerase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.05Å 49.43Å 183.51Å 90.00° 101.82° 90.00°	Depositor
Resolution (Å)	27.17 – 2.89 29.94 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.17-2.89) 99.9 (29.94-2.89)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 2.90Å)	Xtrriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.211 , 0.286 0.226 , 0.299	Depositor DCC
$R_{free}$ test set	1747 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.9	Xtrriage
Anisotropy	0.516	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.51	0/2787	0.70	0/3762
1	B	0.55	0/2787	0.69	0/3762
1	C	0.50	0/2787	0.70	0/3762
1	D	0.52	0/2787	0.71	0/3762
All	All	0.52	0/11148	0.70	0/15048

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2735	0	2771	37	0
1	B	2735	0	2771	21	0
1	C	2735	0	2771	38	0
1	D	2735	0	2771	33	0
2	A	12	0	8	1	0
2	B	12	0	8	0	0
2	C	12	0	8	1	0
2	D	12	0	8	0	0
All	All	10988	0	11116	127	0

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 6.

All (127) 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:A:940:LYS:HG3	1:A:940:LYS:O	1.55	1.02
1:D:823:ALA:HB3	1:D:826:HIS:HD2	1.39	0.86
1:D:830:ASP:HB2	1:D:1008:ASN:HB2	1.70	0.73
1:D:823:ALA:HB3	1:D:826:HIS:CD2	2.24	0.72
1:A:834:ILE:HD11	1:A:1006:LYS:HB2	1.74	0.69
1:A:865:ARG:HD3	1:A:909:HIS:HB2	1.76	0.68
1:B:834:ILE:HD11	1:B:1006:LYS:HB2	1.75	0.68
1:C:919:ILE:HG22	1:C:1003:LEU:HB2	1.75	0.68
1:D:919:ILE:HG22	1:D:1003:LEU:HB2	1.77	0.66
1:B:859:LEU:HG	1:B:921:LEU:HD22	1.79	0.64
1:B:832:GLU:HB3	1:B:1006:LYS:HB3	1.77	0.64
1:C:697:PRO:HD2	1:C:700:LYS:HB2	1.81	0.62
1:A:759:GLN:HG3	1:A:887:THR:HG22	1.83	0.60
1:D:697:PRO:HD2	1:D:700:LYS:HB2	1.85	0.59
1:C:955:THR:HG22	1:C:977:SER:HB2	1.83	0.59
1:A:938:ILE:O	1:A:940:LYS:N	2.30	0.59
1:C:712:ILE:O	1:C:716:VAL:HG23	2.04	0.58
1:D:670:GLN:HG2	1:D:790:ILE:HG21	1.86	0.58
1:B:668:PRO:HG2	1:B:803:VAL:HG21	1.86	0.57
1:C:679:VAL:HG12	1:C:683:LYS:HE2	1.86	0.57
1:D:727:SER:O	1:D:731:ASP:HB2	2.04	0.57
1:B:854:LEU:O	1:B:857:ARG:HD3	2.05	0.56
1:A:903:LYS:HE2	2:A:1101:MEW:H6	1.88	0.56
1:A:686:MET:CB	1:A:693:LEU:HD11	2.36	0.56
1:B:826:HIS:ND1	1:B:902:SER:HB3	2.20	0.56
1:A:956:PRO:HG2	1:A:970:PRO:HB2	1.89	0.55
1:C:788:ASP:HB3	1:C:791:ASP:HB2	1.87	0.55
1:A:798:LYS:O	1:A:842:GLU:HB2	2.06	0.55
1:C:769:LEU:O	1:C:773:VAL:HG23	2.08	0.55
1:C:860:LEU:HD12	1:C:924:VAL:CG2	2.37	0.54
1:C:860:LEU:HD12	1:C:924:VAL:HG21	1.89	0.54
1:A:854:LEU:O	1:A:857:ARG:HD3	2.08	0.54
1:B:697:PRO:HD2	1:B:700:LYS:HB2	1.88	0.54
1:B:706:ILE:HG23	1:B:765:LEU:HD22	1.90	0.54
1:A:832:GLU:HB3	1:A:1006:LYS:HB3	1.90	0.53
1:B:844:GLU:HG2	1:B:998:ASN:HD22	1.74	0.53
1:B:993:ASP:HB3	1:B:996:GLN:HG3	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:669:VAL:O	1:D:673:ILE:HG12	2.09	0.52
1:A:919:ILE:HG22	1:A:1003:LEU:HB2	1.92	0.52
1:C:696:MET:HB2	1:C:741:PRO:HD2	1.92	0.52
1:D:923:GLU:OE2	1:D:967:VAL:CG2	2.57	0.51
1:B:725:SER:HB3	1:D:827:ASN:OD1	2.10	0.51
1:C:821:THR:HB	1:C:900:MET:HA	1.92	0.51
1:D:923:GLU:OE2	1:D:967:VAL:HG21	2.11	0.51
1:A:748:LYS:HD3	1:A:749:PRO:HD2	1.92	0.50
1:B:809:GLU:O	1:B:813:ILE:HG12	2.11	0.50
1:D:903:LYS:NZ	1:D:988:GLU:HG2	2.25	0.50
1:B:687:VAL:HG22	1:B:693:LEU:HD11	1.94	0.50
1:B:801:ILE:HG13	1:B:839:ILE:HG22	1.93	0.50
1:A:940:LYS:CG	1:A:940:LYS:O	2.37	0.50
1:D:809:GLU:O	1:D:813:ILE:HG12	2.12	0.49
1:A:938:ILE:C	1:A:940:LYS:H	2.14	0.49
1:C:801:ILE:HG13	1:C:839:ILE:HG22	1.95	0.49
1:A:872:ILE:HG21	1:A:920:LEU:HD11	1.95	0.49
1:C:920:LEU:HD22	1:C:999:LEU:HD22	1.95	0.49
1:A:895:ILE:HD11	1:A:994:ILE:HG22	1.94	0.48
1:D:858:ARG:HG3	1:D:968:ASP:HB2	1.95	0.48
1:D:962:ILE:HD13	1:D:971:LEU:HD11	1.94	0.48
1:D:930:TYR:CE2	1:D:932:LEU:HD21	2.49	0.48
1:D:683:LYS:O	1:D:687:VAL:HG23	2.13	0.48
1:C:826:HIS:CD2	1:C:902:SER:OG	2.66	0.48
1:D:921:LEU:HB2	1:D:1001:TYR:HB2	1.94	0.48
1:B:828:ALA:HB2	1:D:726:ASP:HB3	1.96	0.47
1:A:962:ILE:HG22	1:A:969:VAL:HB	1.96	0.47
1:C:805:ASP:HB3	1:C:808:SER:HB3	1.96	0.47
1:A:890:MET:HG2	1:A:935:ALA:HA	1.96	0.47
1:C:683:LYS:O	1:C:687:VAL:HG23	2.14	0.47
1:C:869:PHE:HA	1:C:872:ILE:HB	1.96	0.47
1:C:678:ASP:HB3	1:C:681:SER:HB2	1.95	0.47
1:C:814:ILE:HD13	1:C:836:ILE:HG21	1.95	0.47
1:D:770:ASP:OD1	1:D:878:ARG:NH2	2.48	0.47
1:C:854:LEU:O	1:C:857:ARG:HD3	2.15	0.46
1:D:682:MET:O	1:D:686:MET:HG3	2.16	0.46
1:A:863:GLY:N	1:A:904:SER:HB3	2.30	0.45
1:B:919:ILE:HG22	1:B:1003:LEU:HB2	1.98	0.45
1:A:881:PRO:HB2	1:A:883:GLU:OE1	2.17	0.45
1:C:865:ARG:HD3	1:C:909:HIS:HB2	1.99	0.45
1:D:703:LYS:HB2	1:D:704:ARG:HH11	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:LEU:HB3	1:A:1002:LEU:HD21	1.99	0.44
1:A:938:ILE:C	1:A:940:LYS:N	2.70	0.44
1:C:701:LEU:HD21	1:C:768:LEU:HD22	1.99	0.44
1:C:673:ILE:HD11	1:C:794:TYR:HD1	1.83	0.44
1:A:962:ILE:HD12	1:A:971:LEU:HD11	1.99	0.44
1:A:724:SER:HB2	1:A:729:ILE:HD12	1.99	0.44
1:A:670:GLN:HG2	1:A:790:ILE:HG21	1.98	0.44
1:A:931:GLU:HG2	1:A:949:LYS:HB3	2.00	0.44
1:D:859:LEU:HA	1:D:922:GLY:O	2.18	0.44
1:C:903:LYS:HE2	2:C:1101:MEW:H6	2.00	0.43
1:C:869:PHE:O	1:C:873:LEU:HG	2.17	0.43
1:A:804:VAL:HG22	1:A:838:LYS:HB2	2.00	0.43
1:C:797:LEU:HD22	1:C:873:LEU:HB2	2.01	0.43
1:C:863:GLY:HA3	1:C:904:SER:O	2.18	0.43
1:C:879:ILE:HG12	1:C:894:GLY:HA2	2.01	0.43
1:B:767:ASN:HD21	1:B:865:ARG:HG3	1.83	0.43
1:D:699:GLY:O	1:D:700:LYS:HD3	2.19	0.43
1:D:918:LEU:HA	1:D:1003:LEU:O	2.19	0.43
1:D:962:ILE:HG22	1:D:969:VAL:HB	2.00	0.43
1:A:770:ASP:HB3	1:A:868:ASN:HA	2.00	0.42
1:C:902:SER:HA	1:C:905:ALA:HB3	2.01	0.42
1:A:686:MET:CE	1:A:693:LEU:HD11	2.49	0.42
1:A:821:THR:HB	1:A:900:MET:HA	2.02	0.42
1:D:862:HIS:HD2	1:D:896:TYR:O	2.01	0.42
1:B:890:MET:HE1	1:B:983:SER:HB2	2.02	0.42
1:D:676:ILE:HD11	1:D:797:LEU:HD11	2.01	0.42
1:D:931:GLU:HB3	1:D:951:LEU:HD11	2.02	0.42
1:C:701:LEU:HD22	1:C:706:ILE:HD11	2.01	0.42
1:C:921:LEU:HA	1:C:921:LEU:HD23	1.95	0.42
1:D:794:TYR:HA	1:D:797:LEU:HD12	2.01	0.42
1:C:921:LEU:HB2	1:C:1001:TYR:HB2	2.01	0.41
1:C:680:GLU:HA	1:C:683:LYS:HE3	2.01	0.41
1:D:862:HIS:HB3	1:D:920:LEU:HB2	2.03	0.41
1:A:895:ILE:O	1:A:990:ILE:HA	2.20	0.41
1:C:677:PHE:CD1	1:C:778:LEU:HD13	2.56	0.41
1:B:712:ILE:O	1:B:716:VAL:HG23	2.20	0.41
1:A:686:MET:HB2	1:A:693:LEU:HD11	2.02	0.41
1:A:863:GLY:HA3	1:A:904:SER:O	2.21	0.41
1:B:854:LEU:O	1:B:857:ARG:CD	2.69	0.41
1:C:895:ILE:HD11	1:C:994:ILE:HG22	2.02	0.41
1:C:826:HIS:CE1	1:C:906:ASN:HD21	2.39	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:PHE:CE1	1:C:924:VAL:HG11	2.55	0.41
1:C:837:PHE:HB2	1:C:1002:LEU:HB3	2.03	0.41
1:D:682:MET:HB3	1:D:698:LEU:HD21	2.02	0.41
1:A:724:SER:HB3	1:A:728:GLN:HG3	2.03	0.40
1:D:941:LEU:HA	1:D:942:PRO:HD3	1.98	0.40
1:B:797:LEU:HD22	1:B:873:LEU:HB2	2.04	0.40
1:A:859:LEU:HG	1:A:921:LEU:HD22	2.04	0.40
1:A:993:ASP:HB3	1:A:996:GLN:HG3	2.04	0.40

There are no symmetry-related clashes.

## 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	A	346/358 (97%)	325 (94%)	20 (6%)	1 (0%)	41	71
1	B	346/358 (97%)	327 (94%)	19 (6%)	0	100	100
1	C	346/358 (97%)	319 (92%)	23 (7%)	4 (1%)	13	40
1	D	346/358 (97%)	318 (92%)	27 (8%)	1 (0%)	41	71
All	All	1384/1432 (97%)	1289 (93%)	89 (6%)	6 (0%)	34	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	939	SER
1	C	823	ALA
1	C	779	ARG
1	C	939	SER
1	D	867	THR
1	C	824	THR

### 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	305/314 (97%)	280 (92%)	25 (8%)	11	32
1	B	305/314 (97%)	272 (89%)	33 (11%)	6	20
1	C	305/314 (97%)	273 (90%)	32 (10%)	7	21
1	D	305/314 (97%)	277 (91%)	28 (9%)	9	27
All	All	1220/1256 (97%)	1102 (90%)	118 (10%)	8	25

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	664	LYS
1	A	674	LYS
1	A	680	GLU
1	A	694	GLN
1	A	698	LEU
1	A	729	ILE
1	A	731	ASP
1	A	738	THR
1	A	746	MET
1	A	756	ASP
1	A	767	ASN
1	A	778	LEU
1	A	805	ASP
1	A	810	GLU
1	A	817	TYR
1	A	916	ILE
1	A	938	ILE
1	A	941	LEU
1	A	943	LYS
1	A	962	ILE
1	A	964	LEU
1	A	968	ASP
1	A	976	SER
1	A	981	ASP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	985	LEU
1	B	667	LYS
1	B	693	LEU
1	B	700	LYS
1	B	703	LYS
1	B	722	GLN
1	B	728	GLN
1	B	732	LEU
1	B	746	MET
1	B	748	LYS
1	B	757	SER
1	B	758	VAL
1	B	763	GLU
1	B	791	ASP
1	B	805	ASP
1	B	817	TYR
1	B	830	ASP
1	B	838	LYS
1	B	852	LYS
1	B	864	SER
1	B	865	ARG
1	B	875	GLN
1	B	938	ILE
1	B	940	LYS
1	B	959	SER
1	B	963	SER
1	B	964	LEU
1	B	968	ASP
1	B	971	LEU
1	B	980	ASN
1	B	981	ASP
1	B	984	LEU
1	B	985	LEU
1	B	991	VAL
1	C	681	SER
1	C	698	LEU
1	C	701	LEU
1	C	704	ARG
1	C	721	SER
1	C	724	SER
1	C	725	SER
1	C	730	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	731	ASP
1	C	733	SER
1	C	747	LYS
1	C	748	LYS
1	C	769	LEU
1	C	788	ASP
1	C	797	LEU
1	C	812	GLU
1	C	817	TYR
1	C	830	ASP
1	C	831	LEU
1	C	836	ILE
1	C	841	ARG
1	C	852	LYS
1	C	867	THR
1	C	938	ILE
1	C	949	LYS
1	C	962	ILE
1	C	965	ASP
1	C	973	THR
1	C	975	ILE
1	C	976	SER
1	C	985	LEU
1	C	998	ASN
1	D	694	GLN
1	D	710	TYR
1	D	731	ASP
1	D	732	LEU
1	D	733	SER
1	D	735	ARG
1	D	767	ASN
1	D	771	ILE
1	D	778	LEU
1	D	783	ASP
1	D	791	ASP
1	D	795	GLU
1	D	841	ARG
1	D	844	GLU
1	D	845	CYS
1	D	858	ARG
1	D	875	GLN
1	D	886	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	887	THR
1	D	889	TYR
1	D	919	ILE
1	D	940	LYS
1	D	943	LYS
1	D	949	LYS
1	D	962	ILE
1	D	973	THR
1	D	979	VAL
1	D	981	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	722	GLN
1	A	906	ASN
1	B	670	GLN
1	B	722	GLN
1	B	767	ASN
1	C	822	HIS
1	C	826	HIS
1	C	906	ASN
1	C	961	ASN
1	C	998	ASN
1	D	862	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 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	MEW	A	1101	-	12,13,13	1.74	2 (16%)	15,18,18	3.23	8 (53%)
2	MEW	D	1101	-	12,13,13	2.03	4 (33%)	15,18,18	3.12	10 (66%)
2	MEW	B	1101	-	12,13,13	1.75	4 (33%)	15,18,18	3.21	6 (40%)
2	MEW	C	1101	-	12,13,13	2.54	4 (33%)	15,18,18	2.85	9 (60%)

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	MEW	A	1101	-	-	-	0/2/2/2
2	MEW	D	1101	-	-	-	0/2/2/2
2	MEW	B	1101	-	-	-	0/2/2/2
2	MEW	C	1101	-	-	-	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	MEW	CAT-NAQ	5.53	1.43	1.34
2	D	1101	MEW	CAU-NAQ	4.59	1.41	1.33
2	C	1101	MEW	CAU-NAQ	4.53	1.40	1.33
2	A	1101	MEW	CAU-NAQ	3.71	1.39	1.33
2	A	1101	MEW	CAT-NAQ	3.61	1.40	1.34
2	B	1101	MEW	CAU-NAQ	3.54	1.39	1.33
2	D	1101	MEW	CAT-NAQ	3.29	1.39	1.34
2	C	1101	MEW	CAT-NAO	3.18	1.39	1.34
2	B	1101	MEW	CAT-NAQ	3.11	1.39	1.34
2	C	1101	MEW	CAG-CAK	2.68	1.42	1.36
2	D	1101	MEW	CAT-NAO	2.25	1.38	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	MEW	OAC-CAU	-2.18	1.19	1.24
2	D	1101	MEW	CAV-NAO	2.09	1.41	1.37
2	B	1101	MEW	CAH-CAL	2.09	1.41	1.36

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	MEW	CAT-NAO-CAV	7.00	121.29	116.54
2	A	1101	MEW	CAT-NAO-CAV	6.88	121.21	116.54
2	D	1101	MEW	CAW-CAU-NAQ	-6.17	120.10	124.40
2	A	1101	MEW	CAW-CAV-NAO	-5.97	120.36	123.60
2	B	1101	MEW	CAW-CAV-NAO	-5.68	120.52	123.60
2	A	1101	MEW	CAW-CAU-NAQ	-5.66	120.46	124.40
2	B	1101	MEW	CAW-CAU-NAQ	-5.58	120.51	124.40
2	C	1101	MEW	CAT-NAO-CAV	5.28	120.12	116.54
2	C	1101	MEW	CAW-CAU-NAQ	-4.53	121.25	124.40
2	D	1101	MEW	CAN-CAT-NAO	4.28	123.82	117.16
2	D	1101	MEW	CAT-NAO-CAV	4.01	119.26	116.54
2	B	1101	MEW	CAN-CAT-NAQ	3.89	123.22	117.15
2	C	1101	MEW	NAO-CAT-NAQ	-3.88	118.58	125.72
2	D	1101	MEW	NAO-CAT-NAQ	-3.69	118.94	125.72
2	C	1101	MEW	CAW-CAV-NAO	-3.58	121.66	123.60
2	B	1101	MEW	NAO-CAT-NAQ	-3.54	119.21	125.72
2	D	1101	MEW	CAL-CAW-CAV	3.51	122.66	117.55
2	A	1101	MEW	NAO-CAT-NAQ	-3.28	119.69	125.72
2	D	1101	MEW	CAH-CAG-CAK	3.27	125.02	120.44
2	D	1101	MEW	CAK-CAV-CAW	-3.19	115.66	120.05
2	C	1101	MEW	CAG-CAH-CAL	-3.14	116.03	120.44
2	D	1101	MEW	CAW-CAV-NAO	-3.02	121.96	123.60
2	C	1101	MEW	CAL-CAW-CAV	2.95	121.84	117.55
2	D	1101	MEW	CAG-CAH-CAL	-2.85	116.44	120.44
2	A	1101	MEW	CAH-CAL-CAW	-2.77	116.20	120.86
2	A	1101	MEW	CAN-CAT-NAQ	2.67	121.32	117.15
2	C	1101	MEW	CAN-CAT-NAO	2.60	121.20	117.16
2	A	1101	MEW	CAG-CAH-CAL	2.59	124.07	120.44
2	B	1101	MEW	CAL-CAW-CAV	2.48	121.16	117.55
2	D	1101	MEW	CAK-CAV-NAO	2.42	122.38	118.69
2	C	1101	MEW	CAK-CAV-CAW	-2.37	116.79	120.05
2	C	1101	MEW	CAH-CAG-CAK	2.36	123.75	120.44
2	A	1101	MEW	CAL-CAW-CAV	2.36	120.99	117.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	MEW	1	0
2	C	1101	MEW	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	348/358 (97%)	-0.24	4 (1%) 80 80	21, 48, 77, 112	0
1	B	348/358 (97%)	-0.09	9 (2%) 56 52	25, 52, 93, 130	0
1	C	348/358 (97%)	0.18	13 (3%) 41 37	36, 66, 107, 138	0
1	D	348/358 (97%)	0.28	18 (5%) 27 23	37, 68, 97, 134	0
All	All	1392/1432 (97%)	0.03	44 (3%) 47 43	21, 60, 97, 138	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	783	ASP	5.9
1	B	784	ASP	5.7
1	C	783	ASP	5.0
1	D	783	ASP	4.8
1	D	784	ASP	4.7
1	D	980	ASN	4.5
1	D	887	THR	3.9
1	D	781	GLY	3.9
1	A	783	ASP	3.6
1	C	785	SER	3.5
1	C	784	ASP	3.4
1	A	939	SER	3.4
1	D	788	ASP	3.3
1	D	939	SER	3.2
1	C	786	SER	3.2
1	D	782	SER	3.2
1	B	913	GLY	2.8
1	C	782	SER	2.7
1	C	791	ASP	2.7
1	D	882	PRO	2.7
1	A	781	GLY	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	938	ILE	2.7
1	D	746	MET	2.6
1	D	785	SER	2.6
1	C	781	GLY	2.6
1	C	937	HIS	2.6
1	D	704	ARG	2.6
1	D	795	GLU	2.5
1	B	912	GLN	2.5
1	A	746	MET	2.4
1	B	787	LYS	2.4
1	D	789	PRO	2.4
1	D	694	GLN	2.3
1	B	1008	ASN	2.3
1	D	670	GLN	2.3
1	C	664	LYS	2.3
1	B	830	ASP	2.2
1	C	966	GLY	2.2
1	B	785	SER	2.2
1	B	939	SER	2.2
1	C	687	VAL	2.1
1	C	887	THR	2.1
1	C	795	GLU	2.1
1	D	674	LYS	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MEW	D	1101	12/12	0.93	0.17	21,30,35,38	0
2	MEW	B	1101	12/12	0.95	0.18	35,39,40,40	0
2	MEW	C	1101	12/12	0.95	0.20	26,39,40,42	0
2	MEW	A	1101	12/12	0.96	0.18	30,33,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.