



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:58 AM GMT

PDB ID : 2VHF  
Title : STRUCTURE OF THE CYLD USP DOMAIN  
Authors : Komander, D.; Lord, C.J.; Scheel, H.; Swift, S.; Hofmann, K.; Ashworth, A.; Barford, D.  
Deposited on : 2007-11-21  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

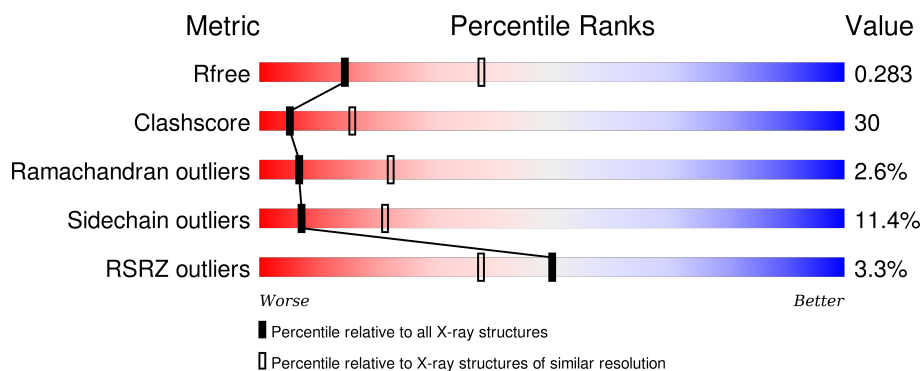
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

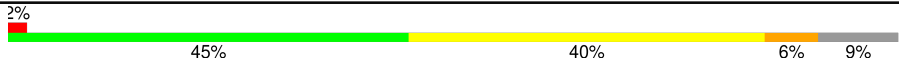
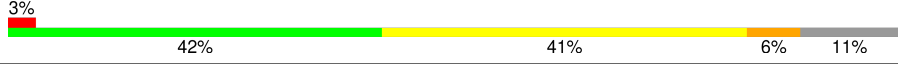
The reported resolution of this entry is 2.80 Å.

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	374	 2% 45% 40% 6% 9%
1	B	374	 3% 42% 41% 6% 11%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5265 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 UBIQUITIN CARBOXYL-TERMINAL HYDROLASE CYLD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2653	1702	443	481	27			
1	B	334	Total	C	N	O	S	0	0	0
			2594	1665	427	475	27			

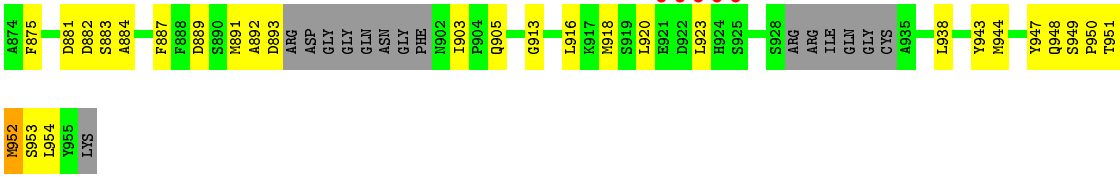
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	5	Total	O	0	0
			5	5		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.49 Å 89.08 Å 171.81 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.80 29.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.79-2.80) 99.1 (29.79-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.233 , 0.281 0.239 , 0.283	Depositor DCC
$R_{free}$ test set	764 reflections (3.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.5	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 62.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 23373 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN

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	0.46	1/2709 (0.0%)	0.56	0/3665
1	B	0.41	1/2651 (0.0%)	0.55	0/3597
All	All	0.44	2/5360 (0.0%)	0.56	0/7262

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	798	GLU	CD-OE2	7.02	1.33	1.25
1	B	798	GLU	CD-OE2	6.81	1.33	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	A	2653	0	2542	141	0
1	B	2594	0	2480	172	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	0	0	0
3	B	5	0	0	0	0
All	All	5265	0	5022	310	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 30.

All (310) 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:B:616:VAL:CA	1:B:952:MET:CE	1.93	1.45
1:B:616:VAL:HA	1:B:952:MET:CE	0.99	1.45
1:B:730:ILE:HD11	1:B:756:MET:CE	1.68	1.24
1:B:827:HIS:HB3	1:B:830:ARG:HH12	1.06	1.21
1:B:616:VAL:HA	1:B:952:MET:HE3	1.20	1.18
1:A:779:ASP:HA	1:A:786:ARG:HD3	1.20	1.15
1:B:730:ILE:HD11	1:B:756:MET:HE1	1.24	1.10
1:B:616:VAL:HA	1:B:952:MET:HE1	1.34	1.08
1:B:830:ARG:HG2	1:B:830:ARG:HH11	0.94	1.06
1:B:616:VAL:CA	1:B:952:MET:HE2	1.71	1.04
1:A:632:TYR:N	1:A:632:TYR:HD2	1.60	1.00
1:A:789:ARG:HH21	1:A:812:LYS:HB3	1.26	0.97
1:A:915:TYR:O	1:A:918:MET:HG3	1.66	0.94
1:B:730:ILE:CD1	1:B:756:MET:HE1	1.98	0.94
1:B:615:SER:O	1:B:952:MET:HE1	1.69	0.92
1:A:632:TYR:N	1:A:632:TYR:CD2	2.30	0.92
1:B:730:ILE:HD11	1:B:756:MET:HE3	1.50	0.92
1:A:616:VAL:HG13	1:A:952:MET:HG2	1.53	0.91
1:B:827:HIS:HB3	1:B:830:ARG:NH1	1.86	0.91
1:A:632:TYR:H	1:A:632:TYR:HD2	1.11	0.90
1:A:729:THR:HB	1:A:732:GLN:HG3	1.52	0.90
1:B:830:ARG:HG2	1:B:830:ARG:NH1	1.75	0.88
1:B:616:VAL:CA	1:B:952:MET:HE3	1.80	0.87
1:B:616:VAL:HA	1:B:952:MET:HE2	0.86	0.85
1:A:614:SER:OG	1:A:616:VAL:HG22	1.78	0.84
1:B:616:VAL:N	1:B:952:MET:HE3	1.93	0.83
1:A:936:ARG:HH11	1:A:936:ARG:HG2	1.41	0.83
1:A:789:ARG:NH2	1:A:812:LYS:HB3	1.93	0.82
1:A:595:GLN:HA	1:A:904:PRO:HG3	1.61	0.81
1:B:827:HIS:CB	1:B:830:ARG:HH12	1.92	0.80
1:B:793:GLY:CA	1:B:851:HIS:HD2	1.95	0.79
1:B:646:ASN:O	1:B:650:ILE:HG13	1.81	0.78
1:B:730:ILE:HG12	1:B:771:PRO:HA	1.65	0.78
1:A:931:ILE:HD11	1:A:936:ARG:HA	1.65	0.78
1:B:769:ILE:O	1:B:771:PRO:HD3	1.84	0.77
1:B:730:ILE:CD1	1:B:756:MET:CE	2.56	0.76
1:B:697:GLU:CD	1:B:697:GLU:H	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:ARG:CG	1:B:830:ARG:HH11	1.85	0.76
1:B:669:VAL:HG21	1:B:693:ILE:HD11	1.67	0.76
1:B:699:LEU:HB2	1:B:713:TYR:HA	1.68	0.75
1:B:633:TYR:O	1:B:637:GLN:HB2	1.86	0.75
1:B:680:LYS:NZ	1:B:681:ASP:HB2	2.02	0.74
1:B:639:LEU:HD12	1:B:643:GLU:HB2	1.69	0.74
1:B:843:ASP:O	1:B:846:ASP:HB2	1.87	0.74
1:B:615:SER:O	1:B:952:MET:CE	2.36	0.73
1:A:918:MET:HB2	1:A:923:LEU:HD21	1.69	0.73
1:A:786:ARG:HH11	1:A:815:GLN:HE21	1.36	0.73
1:A:863:ALA:HB3	1:A:946:MET:HG3	1.71	0.73
1:B:621:LEU:HD22	1:B:641:ARG:HA	1.69	0.73
1:A:878:TYR:HD2	1:A:886:LEU:HG	1.54	0.72
1:B:640:LEU:O	1:B:645:VAL:HG23	1.89	0.71
1:A:878:TYR:CD2	1:A:886:LEU:HG	2.25	0.71
1:B:616:VAL:N	1:B:952:MET:CE	2.53	0.71
1:B:788:CYS:SG	1:B:816:PHE:HA	2.30	0.71
1:B:881:ASP:HB3	1:B:884:ALA:HB2	1.71	0.71
1:A:684:GLU:O	1:A:688:ILE:HG22	1.90	0.70
1:A:779:ASP:CA	1:A:786:ARG:HD3	2.12	0.69
1:B:773:LEU:HD11	1:B:916:LEU:HD13	1.72	0.69
1:B:602:TYR:HB2	1:B:682:PRO:HD3	1.73	0.69
1:A:919:SER:O	1:A:922:ASP:HB2	1.91	0.69
1:B:730:ILE:CG1	1:B:771:PRO:HA	2.23	0.68
1:B:680:LYS:HG2	1:B:681:ASP:N	2.07	0.68
1:A:786:ARG:NH1	1:A:815:GLN:HE21	1.92	0.68
1:B:918:MET:HB2	1:B:923:LEU:HD13	1.75	0.68
1:A:588:ILE:HG23	1:A:908:PRO:HD3	1.74	0.67
1:B:634:SER:O	1:B:638:GLU:HB2	1.94	0.67
1:A:786:ARG:HH11	1:A:815:GLN:NE2	1.92	0.67
1:B:716:GLN:HB2	1:B:755:GLN:NE2	2.10	0.66
1:B:680:LYS:HZ3	1:B:681:ASP:HB2	1.61	0.66
1:B:951:THR:C	1:B:953:SER:H	1.99	0.66
1:B:687:ASN:O	1:B:691:HIS:HB3	1.95	0.66
1:A:867:ILE:HD13	1:A:872:TYR:CD2	2.31	0.65
1:A:704:SER:O	1:A:707:GLN:HB2	1.96	0.65
1:B:616:VAL:CA	1:B:952:MET:HE1	2.04	0.65
1:A:909:CYS:N	1:A:910:PRO:HD3	2.12	0.65
1:B:793:GLY:HA2	1:B:851:HIS:HD2	1.60	0.65
1:B:949:SER:C	1:B:951:THR:H	2.00	0.65
1:B:646:ASN:HB2	1:B:647:PRO:HD3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:LEU:HD23	1:A:908:PRO:HA	1.78	0.64
1:A:928:SER:O	1:A:936:ARG:HG3	1.97	0.64
1:A:715:TYR:OH	1:A:737:SER:HB3	1.97	0.64
1:B:716:GLN:HA	1:B:755:GLN:HB2	1.80	0.64
1:B:867:ILE:HA	1:B:871:HIS:O	1.98	0.63
1:A:591:LYS:HG2	1:A:653:TYR:CD1	2.33	0.63
1:A:638:GLU:O	1:A:642:THR:HB	1.97	0.63
1:B:808:ILE:O	1:B:814:LYS:HE2	1.99	0.63
1:B:657:THR:HG22	1:B:658:LYS:HD2	1.81	0.63
1:B:738:PHE:CD1	1:B:780:LEU:HD22	2.33	0.63
1:A:788:CYS:HB2	1:A:817:CYS:H	1.64	0.63
1:A:759:PHE:CB	1:A:767:LYS:HE2	2.28	0.63
1:A:704:SER:HB3	1:A:743:LEU:HD23	1.80	0.63
1:B:615:SER:C	1:B:952:MET:CE	2.68	0.62
1:B:615:SER:C	1:B:952:MET:HE3	2.19	0.62
1:A:862:PHE:CE2	1:A:946:MET:HB2	2.34	0.62
1:A:688:ILE:O	1:A:692:HIS:HB2	2.00	0.62
1:B:610:LEU:O	1:B:614:SER:HB3	1.99	0.61
1:A:936:ARG:HG2	1:A:936:ARG:NH1	2.12	0.61
1:A:812:LYS:O	1:A:814:LYS:HE3	2.01	0.61
1:B:658:LYS:HD2	1:B:658:LYS:N	2.15	0.61
1:A:911:GLU:HA	1:A:911:GLU:OE2	2.01	0.61
1:A:590:LYS:HG2	1:A:905:GLN:HG3	1.83	0.60
1:A:657:THR:HG22	1:A:658:LYS:HD2	1.82	0.60
1:A:750:SER:O	1:A:948:GLN:HA	2.02	0.60
1:B:639:LEU:HD12	1:B:643:GLU:CB	2.31	0.60
1:B:640:LEU:HA	1:B:644:ILE:HD12	1.84	0.59
1:B:656:ALA:HA	1:B:659:ILE:HD13	1.83	0.59
1:B:660:MET:O	1:B:664:LYS:HG2	2.01	0.59
1:A:703:ARG:HH11	1:A:782:GLU:CD	2.05	0.59
1:B:611:PHE:HB3	1:B:645:VAL:HG13	1.84	0.59
1:A:640:LEU:HA	1:A:644:ILE:HD12	1.83	0.59
1:A:889:ASP:HB3	1:A:892:ALA:HB2	1.84	0.59
1:B:841:PRO:HD2	1:B:844:LEU:HD12	1.85	0.59
1:B:793:GLY:CA	1:B:851:HIS:CD2	2.84	0.58
1:A:618:ASP:O	1:A:622:LEU:HD13	2.03	0.58
1:B:893:ASP:HB3	1:B:903:ILE:HB	1.86	0.58
1:A:746:ALA:HA	1:A:782:GLU:HG3	1.85	0.58
1:B:666:LEU:HD21	1:B:685:PHE:CE1	2.38	0.58
1:A:799:CYS:HB2	1:A:835:TYR:HB3	1.86	0.57
1:A:616:VAL:CG1	1:A:952:MET:HG2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:THR:HG22	1:A:643:GLU:HG2	1.87	0.57
1:A:776:ASN:HA	1:A:858:ASN:ND2	2.20	0.57
1:A:715:TYR:HE2	1:A:717:ILE:HG22	1.69	0.56
1:B:891:MET:O	1:B:893:ASP:N	2.38	0.56
1:B:775:LEU:HG	1:B:947:TYR:CE2	2.40	0.56
1:B:787:GLN:O	1:B:815:GLN:HG3	2.06	0.56
1:A:911:GLU:C	1:A:913:GLY:H	2.09	0.56
1:A:586:ILE:HG22	1:A:651:TYR:O	2.06	0.55
1:B:736:TRP:O	1:B:739:ILE:HG22	2.07	0.55
1:B:850:ARG:HB3	1:B:853:CYS:HB3	1.87	0.55
1:A:716:GLN:HA	1:A:755:GLN:HB2	1.89	0.55
1:A:760:GLY:HA3	1:A:763:PHE:O	2.07	0.55
1:A:867:ILE:HD13	1:A:872:TYR:CE2	2.41	0.55
1:A:666:LEU:O	1:A:669:VAL:HG13	2.05	0.55
1:B:642:THR:HA	1:B:646:ASN:ND2	2.22	0.54
1:A:588:ILE:CG2	1:A:908:PRO:HD3	2.37	0.54
1:A:608:PHE:O	1:A:612:ALA:HB2	2.07	0.54
1:A:689:LEU:HA	1:A:693:ILE:HD12	1.89	0.54
1:B:610:LEU:HB2	1:B:611:PHE:CD1	2.42	0.54
1:B:586:ILE:HG23	1:B:651:TYR:O	2.08	0.54
1:A:748:ALA:HB2	1:A:781:LEU:HD11	1.90	0.54
1:B:713:TYR:CD1	1:B:713:TYR:N	2.75	0.54
1:B:808:ILE:O	1:B:809:SER:C	2.46	0.54
1:B:806:PRO:HA	1:B:810:ALA:HB2	1.90	0.54
1:B:793:GLY:HA2	1:B:851:HIS:CD2	2.43	0.54
1:B:666:LEU:HD21	1:B:685:PHE:CD1	2.43	0.53
1:A:931:ILE:HD11	1:A:936:ARG:CA	2.36	0.53
1:A:727:VAL:HG23	1:A:768:LYS:O	2.09	0.53
1:A:788:CYS:HB2	1:A:817:CYS:N	2.24	0.53
1:A:718:PHE:HZ	1:A:741:SER:HB2	1.74	0.52
1:B:854:ILE:N	1:B:854:ILE:HD12	2.24	0.52
1:A:802:CYS:HB3	1:A:814:LYS:HG3	1.91	0.52
1:B:602:TYR:HB2	1:B:682:PRO:CD	2.40	0.52
1:A:687:ASN:O	1:A:691:HIS:HB3	2.10	0.52
1:A:915:TYR:C	1:A:918:MET:HG3	2.26	0.52
1:A:776:ASN:HD22	1:A:777:ILE:N	2.07	0.52
1:A:649:ARG:NE	1:A:954:LEU:HD11	2.25	0.51
1:A:828:PRO:HA	1:A:831:LEU:HG	1.91	0.51
1:B:616:VAL:CB	1:B:952:MET:HE2	2.39	0.51
1:B:640:LEU:HD22	1:B:689:LEU:HD21	1.91	0.51
1:A:798:GLU:HG2	1:A:838:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:LEU:C	1:B:586:ILE:H	2.14	0.51
1:B:867:ILE:HG13	1:B:871:HIS:O	2.11	0.51
1:B:738:PHE:CE1	1:B:780:LEU:HB3	2.46	0.50
1:A:729:THR:HG22	1:A:731:GLN:H	1.76	0.50
1:A:591:LYS:HG2	1:A:653:TYR:CE1	2.46	0.50
1:A:798:GLU:HG3	1:A:836:ASN:HD21	1.76	0.50
1:A:667:GLU:HA	1:A:670:GLU:HB3	1.93	0.50
1:B:734:LEU:O	1:B:735:GLU:C	2.49	0.50
1:A:730:ILE:CD1	1:A:771:PRO:HA	2.42	0.50
1:A:873:VAL:HG21	1:A:887:PHE:CE1	2.47	0.50
1:A:683:GLU:OE2	1:A:755:GLN:NE2	2.44	0.50
1:B:873:VAL:HG12	1:B:889:ASP:OD1	2.11	0.50
1:B:729:THR:HA	1:B:770:PHE:O	2.11	0.50
1:B:789:ARG:HG2	1:B:815:GLN:HG2	1.94	0.50
1:B:704:SER:HB3	1:B:743:LEU:HD12	1.94	0.50
1:A:955:TYR:N	1:A:955:TYR:CD2	2.79	0.50
1:A:789:ARG:HH21	1:A:812:LYS:CB	2.12	0.49
1:A:613:PHE:HB3	1:A:955:TYR:HE2	1.77	0.49
1:B:777:ILE:HD12	1:B:781:LEU:HD11	1.93	0.49
1:A:886:LEU:CD2	1:A:908:PRO:HA	2.41	0.49
1:B:847:TRP:O	1:B:849:TRP:CD1	2.65	0.49
1:B:695:ARG:HB3	1:B:695:ARG:NH1	2.28	0.49
1:B:839:SER:O	1:B:840:LEU:HD13	2.13	0.49
1:B:639:LEU:HD12	1:B:643:GLU:CD	2.33	0.49
1:A:825:HIS:CD2	1:A:833:HIS:HB2	2.48	0.49
1:A:728:PRO:HD2	1:A:768:LYS:O	2.12	0.49
1:A:861:LEU:HB2	1:A:947:TYR:CE2	2.47	0.49
1:A:602:TYR:CE2	1:A:603:LEU:HD13	2.48	0.48
1:A:597:HIS:CD2	1:A:656:ALA:HB1	2.48	0.48
1:B:621:LEU:HB3	1:B:641:ARG:HG3	1.95	0.48
1:A:936:ARG:O	1:A:940:CYS:SG	2.71	0.48
1:A:603:LEU:O	1:A:604:ASP:C	2.52	0.48
1:B:610:LEU:HB2	1:B:611:PHE:HD1	1.77	0.48
1:A:714:PHE:HE1	1:A:755:GLN:OE1	1.96	0.48
1:B:739:ILE:O	1:B:739:ILE:HG12	2.13	0.48
1:B:830:ARG:CG	1:B:830:ARG:NH1	2.55	0.48
1:B:681:ASP:HB3	1:B:683:GLU:OE2	2.13	0.48
1:A:622:LEU:HD11	1:B:849:TRP:CE3	2.49	0.48
1:B:841:PRO:HD2	1:B:844:LEU:CD1	2.43	0.48
1:A:936:ARG:NH1	1:A:936:ARG:CG	2.75	0.48
1:B:949:SER:C	1:B:951:THR:N	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:ILE:HG12	1:A:755:GLN:O	2.13	0.48
1:B:787:GLN:HG2	1:B:792:GLY:HA2	1.95	0.48
1:B:793:GLY:N	1:B:851:HIS:HD2	2.11	0.48
1:B:802:CYS:HB3	1:B:814:LYS:HG3	1.96	0.48
1:A:771:PRO:HG2	1:A:938:LEU:HD21	1.95	0.48
1:A:648:LEU:HB2	1:A:654:VAL:CG2	2.44	0.48
1:B:841:PRO:HB2	1:B:844:LEU:HG	1.94	0.47
1:B:951:THR:C	1:B:953:SER:N	2.65	0.47
1:A:788:CYS:SG	1:A:816:PHE:HA	2.54	0.47
1:A:619:THR:CG2	1:B:855:PRO:HG3	2.44	0.47
1:B:835:TYR:CD1	1:B:835:TYR:O	2.67	0.47
1:A:639:LEU:HD12	1:A:643:GLU:HB2	1.95	0.47
1:B:620:VAL:HG13	1:B:694:LEU:HD13	1.96	0.47
1:B:827:HIS:CG	1:B:828:PRO:HD2	2.50	0.47
1:B:949:SER:O	1:B:951:THR:N	2.44	0.47
1:A:825:HIS:HD2	1:A:833:HIS:HB2	1.80	0.47
1:A:951:THR:OG1	1:A:951:THR:O	2.32	0.47
1:B:699:LEU:HD12	1:B:713:TYR:O	2.15	0.47
1:A:889:ASP:O	1:A:892:ALA:HB2	2.14	0.47
1:B:704:SER:HA	1:B:742:ASN:O	2.14	0.47
1:B:875:PHE:CG	1:B:938:LEU:HD13	2.50	0.47
1:A:593:GLY:HA3	1:A:888:PHE:CE1	2.50	0.47
1:A:720:GLU:O	1:A:721:LYS:C	2.54	0.47
1:A:619:THR:HG22	1:B:855:PRO:HG3	1.97	0.47
1:A:630:VAL:HB	1:A:632:TYR:CE2	2.50	0.46
1:B:698:PRO:HB3	1:B:711:ASP:HB3	1.98	0.46
1:B:775:LEU:O	1:B:858:ASN:HA	2.16	0.46
1:B:597:HIS:O	1:B:598:TYR:C	2.52	0.46
1:A:760:GLY:O	1:A:761:LYS:C	2.54	0.46
1:A:730:ILE:HG13	1:A:770:PHE:O	2.15	0.46
1:A:646:ASN:HB2	1:A:647:PRO:HD3	1.98	0.46
1:B:797:TYR:HE1	1:B:818:LYS:HD3	1.80	0.46
1:A:595:GLN:HB3	1:A:656:ALA:HB2	1.98	0.46
1:A:909:CYS:O	1:A:909:CYS:SG	2.73	0.46
1:B:789:ARG:NH1	1:B:812:LYS:HD3	2.32	0.45
1:B:659:ILE:O	1:B:663:ARG:HB2	2.16	0.45
1:B:816:PHE:HB2	1:B:821:ASN:HB2	1.99	0.45
1:B:587:MET:O	1:B:592:LYS:HB3	2.17	0.45
1:B:875:PHE:CD1	1:B:938:LEU:HD13	2.52	0.45
1:B:794:LEU:HD23	1:B:796:MET:CE	2.47	0.45
1:B:702:ILE:HD12	1:B:712:CYS:SG	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:ILE:HG13	1:B:757:PRO:HD3	1.98	0.45
1:B:590:LYS:HG3	1:B:905:GLN:NE2	2.32	0.44
1:A:667:GLU:HA	1:A:670:GLU:CB	2.46	0.44
1:A:703:ARG:NH1	1:A:782:GLU:OE2	2.50	0.44
1:B:586:ILE:O	1:B:592:LYS:HD2	2.17	0.44
1:B:825:HIS:O	1:B:831:LEU:HB3	2.17	0.44
1:B:683:GLU:HG3	1:B:944:MET:CE	2.48	0.43
1:B:748:ALA:HA	1:B:749:PRO:HD2	1.83	0.43
1:A:602:TYR:O	1:A:606:THR:CG2	2.66	0.43
1:B:802:CYS:O	1:B:814:LYS:HG3	2.18	0.43
1:A:935:ALA:O	1:A:936:ARG:C	2.57	0.43
1:A:781:LEU:HD23	1:A:782:GLU:N	2.34	0.43
1:B:818:LYS:O	1:B:822:THR:HG23	2.17	0.43
1:A:626:GLU:O	1:A:628:ASN:N	2.51	0.43
1:B:680:LYS:HZ1	1:B:681:ASP:HB2	1.80	0.43
1:A:798:GLU:HG3	1:A:836:ASN:ND2	2.33	0.43
1:B:883:SER:HB3	1:B:913:GLY:HA3	2.01	0.43
1:A:790:ILE:HB	1:A:820:CYS:SG	2.58	0.43
1:B:875:PHE:CZ	1:B:887:PHE:CD1	3.07	0.43
1:B:601:CYS:C	1:B:603:LEU:H	2.22	0.42
1:A:586:ILE:HG22	1:A:586:ILE:O	2.20	0.42
1:A:669:VAL:O	1:A:670:GLU:C	2.57	0.42
1:A:748:ALA:HA	1:A:749:PRO:HD3	1.91	0.42
1:B:805:ASP:HA	1:B:806:PRO:HD3	1.70	0.42
1:B:741:SER:HB3	1:B:743:LEU:HD13	2.00	0.42
1:B:868:GLU:C	1:B:869:THR:HG1	2.22	0.42
1:B:614:SER:C	1:B:954:LEU:HD12	2.39	0.42
1:B:683:GLU:O	1:B:684:GLU:C	2.57	0.42
1:A:597:HIS:HD2	1:A:656:ALA:HB1	1.83	0.42
1:B:779:ASP:OD2	1:B:789:ARG:NH2	2.52	0.42
1:B:844:LEU:C	1:B:846:ASP:H	2.22	0.42
1:B:597:HIS:HE1	1:B:659:ILE:HG22	1.84	0.42
1:B:824:VAL:HG12	1:B:825:HIS:ND1	2.35	0.42
1:A:736:TRP:N	1:A:736:TRP:CD1	2.87	0.42
1:B:952:MET:HB3	1:B:952:MET:HE3	1.70	0.42
1:B:615:SER:HB3	1:B:954:LEU:HG	2.02	0.42
1:A:622:LEU:CD1	1:A:622:LEU:N	2.83	0.42
1:B:683:GLU:HG3	1:B:944:MET:HE1	2.02	0.41
1:A:703:ARG:NH2	1:A:709:VAL:HG22	2.34	0.41
1:B:825:HIS:C	1:B:827:HIS:H	2.22	0.41
1:A:911:GLU:C	1:A:913:GLY:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:LEU:HA	1:A:775:LEU:HD12	1.85	0.41
1:B:685:PHE:O	1:B:688:ILE:HG22	2.20	0.41
1:B:862:PHE:CE2	1:B:948:GLN:HB3	2.56	0.41
1:B:636:THR:OG1	1:B:665:ILE:HD13	2.21	0.41
1:A:918:MET:HE2	1:A:923:LEU:CD2	2.51	0.41
1:A:669:VAL:CG2	1:A:688:ILE:HG13	2.50	0.41
1:A:731:GLN:O	1:A:732:GLN:C	2.59	0.41
1:B:669:VAL:O	1:B:671:ALA:N	2.54	0.41
1:B:658:LYS:HE2	1:B:661:LYS:NZ	2.35	0.41
1:B:738:PHE:HD1	1:B:780:LEU:HD22	1.81	0.41
1:B:777:ILE:CD1	1:B:781:LEU:HD11	2.50	0.41
1:B:694:LEU:O	1:B:695:ARG:C	2.59	0.41
1:A:909:CYS:N	1:A:910:PRO:CD	2.83	0.41
1:A:788:CYS:CB	1:A:817:CYS:H	2.31	0.41
1:B:756:MET:HB2	1:B:943:TYR:O	2.21	0.40
1:A:776:ASN:CG	1:A:858:ASN:HD21	2.24	0.40
1:B:621:LEU:HD21	1:B:645:VAL:HG21	2.02	0.40
1:B:697:GLU:CD	1:B:697:GLU:N	2.65	0.40
1:B:680:LYS:HG2	1:B:681:ASP:HB2	2.02	0.40
1:A:632:TYR:O	1:A:636:THR:OG1	2.30	0.40
1:A:715:TYR:CE2	1:A:717:ILE:HG22	2.54	0.40
1:A:618:ASP:HA	1:A:621:LEU:HD12	2.02	0.40
1:B:800:ARG:C	1:B:800:ARG:HD3	2.42	0.40
1:B:641:ARG:O	1:B:646:ASN:CG	2.59	0.40
1:A:595:GLN:HA	1:A:904:PRO:CG	2.41	0.40
1:B:680:LYS:NZ	1:B:684:GLU:HB2	2.37	0.40
1:A:593:GLY:N	1:A:652:GLY:O	2.44	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	331/374 (88%)	271 (82%)	53 (16%)	7 (2%)	9	29
1	B	322/374 (86%)	268 (83%)	44 (14%)	10 (3%)	5	17
All	All	653/748 (87%)	539 (82%)	97 (15%)	17 (3%)	7	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	920	LEU
1	A	627	LYS
1	A	705	ALA
1	A	912	VAL
1	B	598	TYR
1	B	892	ALA
1	B	809	SER
1	A	601	CYS
1	A	782	GLU
1	B	855	PRO
1	B	869	THR
1	B	952	MET
1	A	785	PRO
1	B	585	GLU
1	B	950	PRO
1	B	644	ILE
1	A	739	ILE

### 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	281/340 (83%)	243 (86%)	38 (14%)	5	14
1	B	279/340 (82%)	253 (91%)	26 (9%)	11	32
All	All	560/680 (82%)	496 (89%)	64 (11%)	7	21

All (64) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	606	THR
1	A	610	LEU
1	A	616	VAL
1	A	622	LEU
1	A	632	TYR
1	A	657	THR
1	A	663	ARG
1	A	666	LEU
1	A	667	GLU
1	A	669	VAL
1	A	688	ILE
1	A	695	ARG
1	A	697	GLU
1	A	703	ARG
1	A	707	GLN
1	A	711	ASP
1	A	750	SER
1	A	767	LYS
1	A	773	LEU
1	A	776	ASN
1	A	800	ARG
1	A	802	CYS
1	A	804	ASP
1	A	815	GLN
1	A	822	THR
1	A	838	VAL
1	A	858	ASN
1	A	865	LEU
1	A	876	VAL
1	A	890	SER
1	A	891	MET
1	A	907	THR
1	A	931	ILE
1	A	934	CYS
1	A	946	MET
1	A	949	SER
1	A	951	THR
1	A	955	TYR
1	B	586	ILE
1	B	587	MET
1	B	601	CYS
1	B	618	ASP
1	B	634	SER

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Mol	Chain	Res	Type
1	B	637	GLN
1	B	642	THR
1	B	658	LYS
1	B	686	LEU
1	B	703	ARG
1	B	711	ASP
1	B	714	PHE
1	B	738	PHE
1	B	743	LEU
1	B	754	ILE
1	B	756	MET
1	B	800	ARG
1	B	802	CYS
1	B	812	LYS
1	B	819	THR
1	B	823	GLN
1	B	830	ARG
1	B	831	LEU
1	B	839	SER
1	B	840	LEU
1	B	882	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	HIS
1	A	707	GLN
1	A	710	GLN
1	A	776	ASN
1	A	787	GLN
1	A	815	GLN
1	A	821	ASN
1	A	836	ASN
1	A	858	ASN
1	A	905	GLN
1	B	597	HIS
1	B	637	GLN
1	B	716	GLN
1	B	740	ASN
1	B	755	GLN
1	B	821	ASN
1	B	836	ASN

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Mol	Chain	Res	Type
1	B	851	HIS
1	B	905	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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.

No monomer is involved in short contacts.

## 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, 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	341/374 (91%)	0.00	9 (2%) 59 47	26, 54, 97, 133	5 (1%)
1	B	334/374 (89%)	0.16	13 (3%) 43 31	32, 62, 105, 135	9 (2%)
All	All	675/748 (90%)	0.08	22 (3%) 50 38	26, 60, 101, 135	14 (2%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	892	ALA	3.8
1	B	922	ASP	3.8
1	B	605	SER	3.5
1	B	601	CYS	3.3
1	B	587	MET	3.0
1	B	921	GLU	2.9
1	B	709	VAL	2.8
1	B	924	HIS	2.6
1	B	925	SER	2.6
1	A	760	GLY	2.6
1	A	839	SER	2.5
1	B	584	LEU	2.5
1	B	692	HIS	2.4
1	A	583	GLY	2.4
1	B	609	CYS	2.2
1	B	923	LEU	2.2
1	A	926	LEU	2.1
1	A	934	CYS	2.1
1	B	665	ILE	2.1
1	A	726	GLY	2.0
1	A	609	CYS	2.0
1	A	762	ASP	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. 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, 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	1956	1/1	0.99	0.14	-0.74	47,47,47,47	0
2	ZN	A	1957	1/1	0.98	0.13	-1.11	63,63,63,63	0
2	ZN	B	1957	1/1	0.99	0.11	-1.35	67,67,67,67	0
2	ZN	A	1958	1/1	0.99	0.12	-2.04	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.