



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:57 PM GMT

PDB ID : 1Z7L  
Title : Crystal structure of fragment of mouse ubiquitin-activating enzyme  
Authors : Szczepanowski, R.H.; Filipek, R.; Bochtler, M.  
Deposited on : 2005-03-25  
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

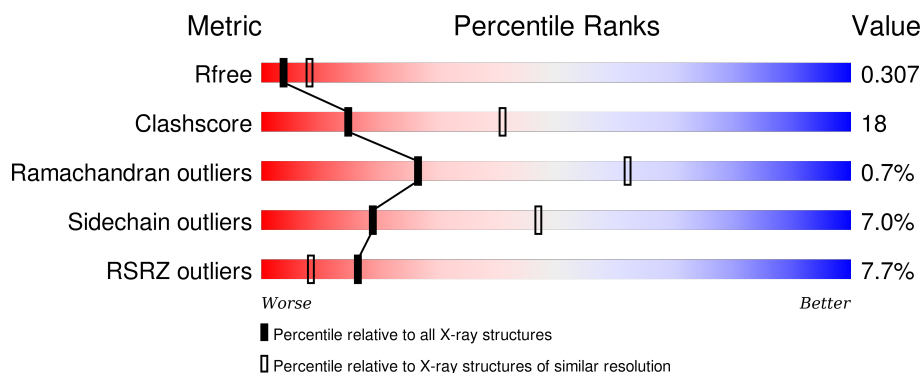
# 1 Overall quality at a glance ⓘ

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	276	<div> <div>8%</div> <div>62% 28% 8%</div> </div>
1	B	276	<div> <div>3%</div> <div>63% 27% 8%</div> </div>
1	C	276	<div> <div>10%</div> <div>62% 28% 8%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6144 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-activating enzyme E1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2030	1287	353	382	8			
1	B	255	Total	C	N	O	S	0	0	0
			2030	1287	353	382	8			
1	C	255	Total	C	N	O	S	0	0	0
			2030	1287	353	382	8			

There are 30 discrepancies between the modelled and reference sequences:

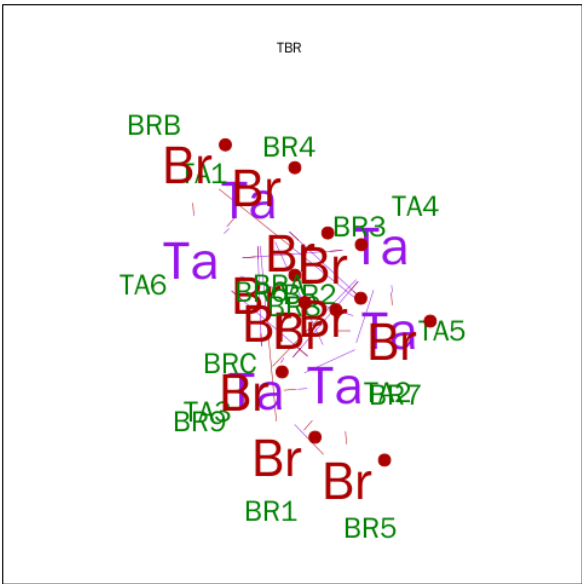
Chain	Residue	Modelled	Actual	Comment	Reference
A	616	MET	-	EXPRESSION TAG	UNP Q02053
A	617	GLY	-	EXPRESSION TAG	UNP Q02053
A	618	HIS	-	EXPRESSION TAG	UNP Q02053
A	619	HIS	-	EXPRESSION TAG	UNP Q02053
A	620	HIS	-	EXPRESSION TAG	UNP Q02053
A	621	HIS	-	EXPRESSION TAG	UNP Q02053
A	622	HIS	-	EXPRESSION TAG	UNP Q02053
A	623	HIS	-	EXPRESSION TAG	UNP Q02053
A	624	GLU	-	EXPRESSION TAG	UNP Q02053
A	625	PHE	-	EXPRESSION TAG	UNP Q02053
B	616	MET	-	EXPRESSION TAG	UNP Q02053
B	617	GLY	-	EXPRESSION TAG	UNP Q02053
B	618	HIS	-	EXPRESSION TAG	UNP Q02053
B	619	HIS	-	EXPRESSION TAG	UNP Q02053
B	620	HIS	-	EXPRESSION TAG	UNP Q02053
B	621	HIS	-	EXPRESSION TAG	UNP Q02053
B	622	HIS	-	EXPRESSION TAG	UNP Q02053
B	623	HIS	-	EXPRESSION TAG	UNP Q02053
B	624	GLU	-	EXPRESSION TAG	UNP Q02053
B	625	PHE	-	EXPRESSION TAG	UNP Q02053
C	616	MET	-	EXPRESSION TAG	UNP Q02053
C	617	GLY	-	EXPRESSION TAG	UNP Q02053
C	618	HIS	-	EXPRESSION TAG	UNP Q02053

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Chain	Residue	Modelled	Actual	Comment	Reference
C	619	HIS	-	EXPRESSION TAG	UNP Q02053
C	620	HIS	-	EXPRESSION TAG	UNP Q02053
C	621	HIS	-	EXPRESSION TAG	UNP Q02053
C	622	HIS	-	EXPRESSION TAG	UNP Q02053
C	623	HIS	-	EXPRESSION TAG	UNP Q02053
C	624	GLU	-	EXPRESSION TAG	UNP Q02053
C	625	PHE	-	EXPRESSION TAG	UNP Q02053

- Molecule 2 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: Br<sub>12</sub>Ta<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Br	Ta	0	0
			18	12	6		
2	B	1	Total	Br	Ta	0	0
			18	12	6		
2	C	1	Total	Br	Ta	0	0
			18	12	6		

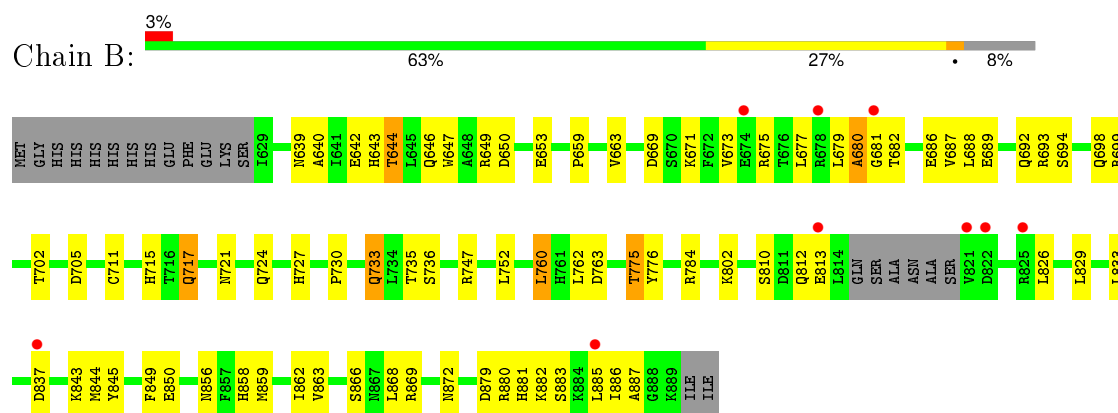
### 3 Residue-property plots

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.

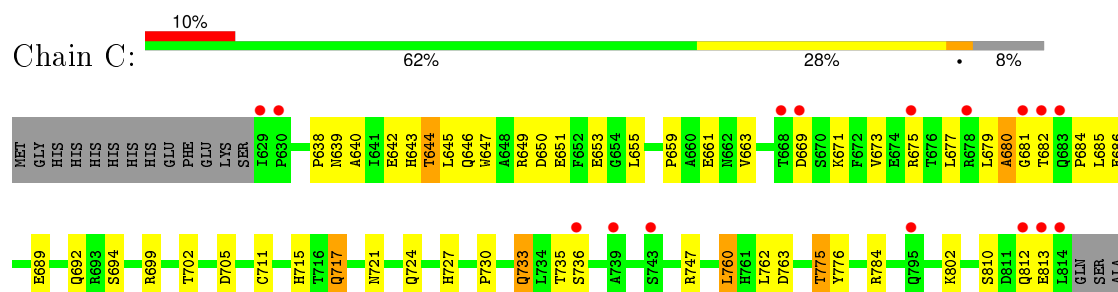
#### • Molecule 1: Ubiquitin-activating enzyme E1 1

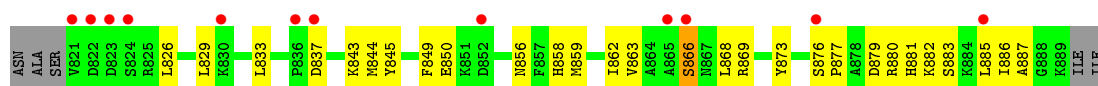


#### • Molecule 1: Ubiquitin-activating enzyme E1 1



#### • Molecule 1: Ubiquitin-activating enzyme E1 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	216.12Å 216.12Å 196.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (10.00-2.80) 99.0 (19.99-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.06 (at 2.79Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.277 , 0.308 0.276 , 0.307	Depositor DCC
$R_{free}$ test set	2109 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.9	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 42745 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: TBR

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	0.41	0/2085	0.65	0/2841
1	B	0.42	0/2085	0.66	0/2841
1	C	0.42	0/2085	0.65	0/2841
All	All	0.42	0/6255	0.65	0/8523

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

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	2030	0	1953	71	0
1	B	2030	0	1953	70	0
1	C	2030	0	1953	72	0
2	A	18	0	0	3	0
2	B	18	0	0	3	0
2	C	18	0	0	2	0
All	All	6144	0	5859	213	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 18.



All (213) 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:717:GLN:HA	1:A:717:GLN:HE21	1.15	1.09
1:B:717:GLN:HE21	1:B:717:GLN:HA	1.20	1.05
1:C:717:GLN:HA	1:C:717:GLN:HE21	1.15	1.03
1:C:649:ARG:HH12	1:C:653:GLU:HG2	1.24	1.01
1:A:649:ARG:HH12	1:A:653:GLU:HG2	1.27	0.98
1:B:649:ARG:HH12	1:B:653:GLU:HG2	1.29	0.97
1:B:639:ASN:H	1:B:643:HIS:HD2	1.15	0.94
1:A:639:ASN:H	1:A:643:HIS:HD2	1.18	0.91
1:C:639:ASN:H	1:C:643:HIS:HD2	1.20	0.89
1:B:881:HIS:O	1:B:885:LEU:HG	1.73	0.88
1:B:671:LYS:HE3	1:B:675:ARG:HD3	1.58	0.86
1:A:671:LYS:HE3	1:A:675:ARG:HD3	1.57	0.86
1:C:671:LYS:HE3	1:C:675:ARG:HD3	1.56	0.85
1:C:881:HIS:O	1:C:885:LEU:HG	1.76	0.84
1:C:649:ARG:NH1	1:C:653:GLU:HG2	1.93	0.83
1:A:717:GLN:HE21	1:A:717:GLN:CA	1.90	0.83
1:C:717:GLN:CA	1:C:717:GLN:HE21	1.92	0.83
1:A:881:HIS:O	1:A:885:LEU:HG	1.80	0.82
1:A:649:ARG:NH1	1:A:653:GLU:HG2	1.97	0.79
1:B:649:ARG:NH1	1:B:653:GLU:HG2	1.97	0.78
1:C:879:ASP:OD1	1:C:882:LYS:HG3	1.83	0.78
1:A:717:GLN:HA	1:A:717:GLN:NE2	1.96	0.78
1:C:735:THR:HG22	1:C:736:SER:H	1.49	0.77
1:B:717:GLN:CA	1:B:717:GLN:HE21	1.95	0.77
1:A:879:ASP:OD1	1:A:882:LYS:HG3	1.84	0.76
1:C:717:GLN:HA	1:C:717:GLN:NE2	1.98	0.76
1:B:879:ASP:OD1	1:B:882:LYS:HG3	1.85	0.75
1:B:730:PRO:HD2	1:B:733:GLN:CG	2.16	0.75
1:C:639:ASN:H	1:C:643:HIS:CD2	2.06	0.73
1:B:717:GLN:NE2	1:B:717:GLN:HA	2.01	0.73
1:B:735:THR:HG22	1:B:736:SER:H	1.53	0.73
1:B:639:ASN:H	1:B:643:HIS:CD2	2.05	0.73
1:C:730:PRO:HD2	1:C:733:GLN:CG	2.19	0.72
1:A:677:LEU:HD11	1:A:826:LEU:HD21	1.72	0.72
1:A:730:PRO:HD2	1:A:733:GLN:CG	2.21	0.71
1:A:735:THR:HG22	1:A:736:SER:H	1.56	0.70
1:A:650:ASP:HA	2:A:999:TBR:BR6	2.46	0.70
1:B:650:ASP:HA	2:B:1000:TBR:BR6	2.45	0.70
1:C:730:PRO:HD2	1:C:733:GLN:HG2	1.72	0.69
1:C:677:LEU:HD11	1:C:826:LEU:HD21	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:PRO:HD2	1:B:733:GLN:HG2	1.74	0.69
1:C:763:ASP:OD1	1:C:784:ARG:NH2	2.26	0.68
1:B:677:LEU:HD11	1:B:826:LEU:HD21	1.76	0.68
1:C:650:ASP:HA	2:C:1001:TBR:BR6	2.48	0.68
1:A:730:PRO:HD2	1:A:733:GLN:HG2	1.76	0.67
1:A:639:ASN:H	1:A:643:HIS:CD2	2.07	0.66
1:C:735:THR:HG22	1:C:736:SER:N	2.11	0.65
1:A:717:GLN:HE22	1:A:721:ASN:HD22	1.43	0.65
1:A:702:THR:HG23	1:A:705:ASP:H	1.61	0.65
1:C:849:PHE:HZ	1:C:859:MET:CE	2.10	0.64
1:C:640:ALA:H	1:C:643:HIS:CD2	2.16	0.64
1:C:702:THR:HG23	1:C:705:ASP:H	1.62	0.64
1:C:717:GLN:HE22	1:C:721:ASN:HD22	1.45	0.63
1:A:849:PHE:HZ	1:A:859:MET:CE	2.12	0.63
1:B:763:ASP:OD1	1:B:784:ARG:NH2	2.31	0.63
1:B:717:GLN:HE22	1:B:721:ASN:HD22	1.47	0.62
1:A:702:THR:HG22	1:A:705:ASP:CG	2.19	0.62
1:C:702:THR:HG22	1:C:705:ASP:CG	2.19	0.62
1:A:763:ASP:OD1	1:A:784:ARG:NH2	2.33	0.62
1:B:735:THR:HG22	1:B:736:SER:N	2.15	0.61
1:B:673:VAL:O	1:B:677:LEU:HB2	2.00	0.60
1:B:849:PHE:HZ	1:B:859:MET:CE	2.14	0.60
1:B:702:THR:HG23	1:B:705:ASP:H	1.65	0.60
1:A:640:ALA:H	1:A:643:HIS:CD2	2.19	0.60
1:B:730:PRO:HD2	1:B:733:GLN:HG3	1.83	0.60
1:C:673:VAL:O	1:C:677:LEU:HB2	2.01	0.60
1:B:702:THR:HG22	1:B:705:ASP:CG	2.22	0.59
1:C:659:PRO:O	1:C:663:VAL:HG23	2.02	0.59
1:B:717:GLN:NE2	1:B:721:ASN:HD22	2.01	0.59
1:A:717:GLN:NE2	1:A:721:ASN:HD22	2.00	0.59
1:B:760:LEU:HD13	1:B:868:LEU:CD2	2.34	0.58
1:B:650:ASP:OD1	2:B:1000:TBR:BR6	2.76	0.58
1:A:760:LEU:HD13	1:A:868:LEU:CD2	2.34	0.57
1:A:735:THR:HG22	1:A:736:SER:N	2.17	0.57
1:A:650:ASP:OD1	2:A:999:TBR:BR6	2.78	0.57
1:B:659:PRO:O	1:B:663:VAL:HG23	2.04	0.57
1:C:640:ALA:H	1:C:643:HIS:HD2	1.52	0.57
1:B:760:LEU:HD13	1:B:868:LEU:HD23	1.85	0.57
1:C:717:GLN:NE2	1:C:721:ASN:HD22	2.03	0.56
1:B:640:ALA:H	1:B:643:HIS:CD2	2.24	0.56
1:C:711:CYS:O	1:C:715:HIS:HD2	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:VAL:O	1:A:677:LEU:HB2	2.05	0.55
1:A:760:LEU:HD13	1:A:868:LEU:HD23	1.88	0.55
1:C:843:LYS:HE2	1:C:845:TYR:OH	2.07	0.55
1:C:862:ILE:O	1:C:866:SER:HB3	2.07	0.55
1:B:682:THR:HG23	1:B:686:GLU:OE1	2.07	0.54
1:A:862:ILE:O	1:A:866:SER:HB3	2.08	0.53
1:A:671:LYS:O	1:A:675:ARG:CB	2.56	0.53
1:B:671:LYS:O	1:B:675:ARG:CB	2.56	0.53
1:A:671:LYS:O	1:A:675:ARG:HB2	2.09	0.53
1:C:730:PRO:HD2	1:C:733:GLN:HG3	1.90	0.53
1:C:671:LYS:O	1:C:675:ARG:CB	2.57	0.52
1:B:671:LYS:O	1:B:675:ARG:HB2	2.09	0.52
1:C:671:LYS:O	1:C:675:ARG:HB2	2.09	0.52
1:C:682:THR:HG23	1:C:686:GLU:OE1	2.10	0.52
1:C:812:GLN:OE1	1:C:812:GLN:HA	2.10	0.52
1:A:730:PRO:HD2	1:A:733:GLN:HG3	1.89	0.52
1:B:812:GLN:OE1	1:B:812:GLN:HA	2.10	0.52
1:A:850:GLU:H	1:A:858:HIS:HD2	1.58	0.51
1:A:812:GLN:OE1	1:A:812:GLN:HA	2.11	0.51
1:A:682:THR:HG23	1:A:686:GLU:OE1	2.10	0.51
1:C:760:LEU:HD13	1:C:868:LEU:HD23	1.91	0.51
1:A:856:ASN:HB3	1:A:858:HIS:ND1	2.26	0.51
1:B:711:CYS:O	1:B:715:HIS:HD2	1.93	0.51
1:A:640:ALA:H	1:A:643:HIS:HD2	1.58	0.51
1:C:760:LEU:HD13	1:C:868:LEU:CD2	2.41	0.51
1:C:882:LYS:O	1:C:886:ILE:HG13	2.11	0.51
1:B:850:GLU:H	1:B:858:HIS:HD2	1.57	0.51
1:C:689:GLU:HG3	1:C:829:LEU:HD11	1.94	0.50
1:C:679:LEU:HD12	1:C:680:ALA:H	1.76	0.50
1:C:650:ASP:OD1	2:C:1001:TBR:BR6	2.85	0.50
1:C:845:TYR:CD1	1:C:845:TYR:N	2.79	0.50
1:B:845:TYR:N	1:B:845:TYR:CD1	2.80	0.50
1:A:845:TYR:N	1:A:845:TYR:CD1	2.79	0.50
1:A:882:LYS:HA	1:A:885:LEU:HD12	1.94	0.49
1:A:711:CYS:O	1:A:715:HIS:HD2	1.94	0.49
1:C:856:ASN:HB3	1:C:858:HIS:ND1	2.28	0.49
1:C:850:GLU:H	1:C:858:HIS:HD2	1.61	0.49
1:B:862:ILE:O	1:B:866:SER:HB3	2.12	0.48
1:A:689:GLU:HG3	1:A:829:LEU:HD11	1.95	0.48
1:B:856:ASN:HB3	1:B:858:HIS:ND1	2.29	0.48
1:C:639:ASN:HA	1:C:747:ARG:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:882:LYS:HA	1:B:885:LEU:HD12	1.94	0.48
1:C:883:SER:O	1:C:887:ALA:HB2	2.14	0.48
1:C:692:GLN:OE1	1:C:833:LEU:HD23	2.14	0.47
1:B:692:GLN:OE1	1:B:833:LEU:HD23	2.14	0.47
1:B:883:SER:O	1:B:887:ALA:HB2	2.14	0.47
1:A:849:PHE:HZ	1:A:859:MET:HE2	1.77	0.47
1:A:752:LEU:HD13	1:A:872:ASN:OD1	2.15	0.47
1:A:659:PRO:O	1:A:663:VAL:HG23	2.15	0.47
1:A:775:THR:HG23	1:A:844:MET:HE2	1.96	0.47
1:A:863:VAL:HG21	1:A:880:ARG:HA	1.97	0.47
1:B:689:GLU:HG3	1:B:829:LEU:HD11	1.96	0.47
1:A:850:GLU:H	1:A:858:HIS:CD2	2.33	0.47
1:A:843:LYS:HE2	1:A:845:TYR:OH	2.14	0.46
1:A:692:GLN:OE1	1:A:833:LEU:HD23	2.15	0.46
1:A:775:THR:HG22	1:A:776:TYR:CD2	2.51	0.46
1:A:883:SER:O	1:A:887:ALA:HB2	2.16	0.46
1:C:876:SER:HA	1:C:877:PRO:HD3	1.82	0.46
1:A:717:GLN:NE2	1:A:717:GLN:CA	2.63	0.45
1:B:850:GLU:H	1:B:858:HIS:CD2	2.33	0.45
1:C:863:VAL:HG21	1:C:880:ARG:HA	1.98	0.45
1:A:702:THR:HG23	1:A:705:ASP:N	2.29	0.45
1:B:858:HIS:O	1:B:862:ILE:HG12	2.17	0.45
1:A:775:THR:HG23	1:A:844:MET:CE	2.47	0.45
1:B:775:THR:HG23	1:B:844:MET:CE	2.46	0.45
1:C:647:TRP:CE3	1:C:869:ARG:HD2	2.52	0.45
1:B:639:ASN:HA	1:B:747:ARG:HD2	1.99	0.45
1:A:644:THR:HG23	1:A:866:SER:HA	1.99	0.44
1:B:679:LEU:HD12	1:B:680:ALA:H	1.82	0.44
1:C:775:THR:HG23	1:C:844:MET:CE	2.47	0.44
1:C:850:GLU:H	1:C:858:HIS:CD2	2.36	0.44
1:B:849:PHE:HZ	1:B:859:MET:HE2	1.82	0.44
1:A:858:HIS:O	1:A:862:ILE:HG12	2.18	0.44
1:B:644:THR:CG2	1:B:866:SER:OG	2.66	0.44
1:A:856:ASN:HB3	1:A:858:HIS:H	1.83	0.44
1:C:702:THR:HG23	1:C:705:ASP:N	2.31	0.43
1:B:775:THR:HG22	1:B:776:TYR:CD2	2.53	0.43
1:A:639:ASN:HA	1:A:747:ARG:HD2	1.99	0.43
1:B:856:ASN:HB3	1:B:858:HIS:H	1.83	0.43
1:C:647:TRP:CD2	1:C:869:ARG:HD2	2.53	0.43
1:C:651:GLU:HG3	1:C:655:LEU:CD1	2.49	0.43
1:C:849:PHE:HZ	1:C:859:MET:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:VAL:HG21	1:B:880:ARG:HA	2.00	0.43
1:C:644:THR:HG23	1:C:866:SER:HA	2.01	0.43
1:C:689:GLU:CG	1:C:829:LEU:HD11	2.49	0.43
1:A:762:LEU:HD23	1:A:762:LEU:HA	1.85	0.43
1:A:679:LEU:HD12	1:A:680:ALA:H	1.84	0.43
1:C:775:THR:HG22	1:C:776:TYR:CD2	2.54	0.43
1:C:724:GLN:O	1:C:727:HIS:HB3	2.19	0.43
1:C:702:THR:HG22	1:C:705:ASP:OD2	2.19	0.43
1:A:810:SER:O	1:A:812:GLN:N	2.51	0.42
1:A:689:GLU:CG	1:A:829:LEU:HD11	2.49	0.42
1:C:858:HIS:O	1:C:862:ILE:HG12	2.19	0.42
1:B:843:LYS:HE2	1:B:845:TYR:OH	2.19	0.42
1:A:718:TYR:HA	1:A:872:ASN:HD21	1.84	0.42
1:B:810:SER:O	1:B:812:GLN:N	2.50	0.42
1:C:685:LEU:HA	1:C:685:LEU:HD23	1.89	0.42
1:C:810:SER:O	1:C:812:GLN:N	2.52	0.42
1:C:638:PRO:HD2	1:C:873:TYR:CE2	2.54	0.42
1:C:640:ALA:N	1:C:643:HIS:CD2	2.87	0.42
1:C:717:GLN:CA	1:C:717:GLN:NE2	2.65	0.42
1:B:886:ILE:O	1:B:886:ILE:HG22	2.19	0.42
1:C:644:THR:HG22	1:C:645:LEU:N	2.35	0.41
1:B:752:LEU:HD13	1:B:872:ASN:OD1	2.20	0.41
1:A:638:PRO:HD2	1:A:873:TYR:CE2	2.56	0.41
1:B:644:THR:HG23	1:B:866:SER:HA	2.02	0.41
1:B:689:GLU:CG	1:B:829:LEU:HD11	2.50	0.41
1:C:849:PHE:CZ	1:C:859:MET:CE	2.97	0.41
1:B:644:THR:HG22	1:B:866:SER:OG	2.21	0.41
1:B:640:ALA:H	1:B:643:HIS:HD2	1.67	0.41
1:A:650:ASP:CG	2:A:999:TBR:BR6	3.14	0.41
1:B:650:ASP:CG	2:B:1000:TBR:BR6	3.14	0.41
1:C:685:LEU:HD23	1:C:826:LEU:HD12	2.02	0.41
1:B:882:LYS:O	1:B:886:ILE:HG13	2.21	0.41
1:A:849:PHE:CZ	1:A:859:MET:HE2	2.56	0.41
1:B:702:THR:HG23	1:B:705:ASP:N	2.32	0.41
1:B:849:PHE:CZ	1:B:859:MET:CE	3.00	0.40
1:C:775:THR:HG23	1:C:844:MET:HE2	2.03	0.40
1:B:687:VAL:HG12	1:B:688:LEU:N	2.36	0.40
1:C:849:PHE:CZ	1:C:859:MET:HE2	2.56	0.40
1:A:693:ARG:HG3	1:A:698:GLN:HG3	2.03	0.40
1:B:671:LYS:O	1:B:671:LYS:HG3	2.21	0.40
1:A:796:VAL:HA	1:A:797:PRO:HD3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:ARG:HG3	1:B:698:GLN:HG3	2.03	0.40
1:A:647:TRP:CE3	1:A:869:ARG:HD2	2.56	0.40
1:B:724:GLN:O	1:B:727:HIS:HB3	2.21	0.40
1:A:849:PHE:CZ	1:A:859:MET:CE	2.99	0.40
1:C:856:ASN:HB3	1:C:858:HIS:H	1.85	0.40
1:A:800:THR:HA	1:A:801:PRO:HD3	1.97	0.40
1:A:644:THR:CG2	1:A:866:SER:OG	2.69	0.40
1:B:647:TRP:CD2	1:B:869:ARG:HD2	2.57	0.40
1:B:647:TRP:CE3	1:B:869:ARG:HD2	2.56	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	251/276 (91%)	232 (92%)	18 (7%)	1 (0%)	39	74
1	B	251/276 (91%)	235 (94%)	14 (6%)	2 (1%)	24	58
1	C	251/276 (91%)	233 (93%)	16 (6%)	2 (1%)	24	58
All	All	753/828 (91%)	700 (93%)	48 (6%)	5 (1%)	26	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	681	GLY
1	B	681	GLY
1	C	681	GLY
1	C	680	ALA
1	B	680	ALA

### 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	223/243 (92%)	207 (93%)	16 (7%)	18	45
1	B	223/243 (92%)	209 (94%)	14 (6%)	22	53
1	C	223/243 (92%)	206 (92%)	17 (8%)	16	42
All	All	669/729 (92%)	622 (93%)	47 (7%)	19	47

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	642	GLU
1	A	644	THR
1	A	646	GLN
1	A	669	ASP
1	A	684	PRO
1	A	694	SER
1	A	699	ARG
1	A	717	GLN
1	A	733	GLN
1	A	760	LEU
1	A	762	LEU
1	A	775	THR
1	A	802	LYS
1	A	813	GLU
1	A	837	ASP
1	A	866	SER
1	B	642	GLU
1	B	644	THR
1	B	646	GLN
1	B	669	ASP
1	B	694	SER
1	B	699	ARG
1	B	717	GLN
1	B	733	GLN
1	B	760	LEU
1	B	762	LEU

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Mol	Chain	Res	Type
1	B	775	THR
1	B	802	LYS
1	B	813	GLU
1	B	837	ASP
1	C	642	GLU
1	C	644	THR
1	C	646	GLN
1	C	661	GLU
1	C	669	ASP
1	C	684	PRO
1	C	694	SER
1	C	699	ARG
1	C	717	GLN
1	C	733	GLN
1	C	760	LEU
1	C	762	LEU
1	C	775	THR
1	C	802	LYS
1	C	813	GLU
1	C	837	ASP
1	C	866	SER

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	643	HIS
1	A	683	GLN
1	A	715	HIS
1	A	717	GLN
1	B	643	HIS
1	B	646	GLN
1	B	715	HIS
1	B	717	GLN
1	C	643	HIS
1	C	715	HIS
1	C	717	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 ⓘ

3 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	TBR	A	999	-	0,36,36	0.00	-	0,180,180	0.00	-
2	TBR	B	1000	-	0,36,36	0.00	-	0,180,180	0.00	-
2	TBR	C	1001	-	0,36,36	0.00	-	0,180,180	0.00	-

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	TBR	A	999	-	-	0/0/696/696	0/0/19/19
2	TBR	B	1000	-	-	0/0/696/696	0/0/19/19
2	TBR	C	1001	-	-	0/0/696/696	0/0/19/19

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.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	TBR	3	0
2	B	1000	TBR	3	0
2	C	1001	TBR	2	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	255/276 (92%)	0.34	22 (8%) 13 6	23, 70, 112, 161	0
1	B	255/276 (92%)	0.15	9 (3%) 48 35	23, 63, 103, 162	0
1	C	255/276 (92%)	0.64	28 (10%) 7 3	23, 81, 117, 162	0
All	All	765/828 (92%)	0.38	59 (7%) 16 8	23, 73, 113, 162	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	821	VAL	7.2
1	B	821	VAL	6.7
1	C	629	ILE	4.4
1	C	812	GLN	4.2
1	B	885	LEU	4.0
1	A	814	LEU	4.0
1	C	823	ASP	3.9
1	C	678	ARG	3.7
1	C	821	VAL	3.7
1	C	830	LYS	3.6
1	B	681	GLY	3.6
1	A	806	LYS	3.6
1	C	885	LEU	3.5
1	C	822	ASP	3.5
1	C	630	PRO	3.5
1	C	668	THR	3.5
1	C	837	ASP	3.4
1	B	822	ASP	3.4
1	C	736	SER	3.4
1	C	743	SER	3.3
1	A	812	GLN	3.2
1	B	678	ARG	3.1
1	C	824	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	825	ARG	3.0
1	C	852	ASP	2.8
1	C	813	GLU	2.8
1	A	809	VAL	2.8
1	A	679	LEU	2.8
1	C	675	ARG	2.8
1	C	681	GLY	2.7
1	A	804	GLY	2.6
1	A	824	SER	2.5
1	C	682	THR	2.5
1	A	670	SER	2.5
1	C	669	ASP	2.5
1	C	739	ALA	2.5
1	B	825	ARG	2.5
1	B	813	GLU	2.5
1	B	837	ASP	2.5
1	C	866	SER	2.3
1	A	745	PRO	2.3
1	A	838	LYS	2.3
1	A	889	LYS	2.3
1	C	876	SER	2.3
1	A	813	GLU	2.3
1	A	810	SER	2.2
1	C	814	LEU	2.2
1	A	823	ASP	2.2
1	A	678	ARG	2.2
1	C	683	GLN	2.2
1	C	795	GLN	2.2
1	A	798	GLU	2.1
1	A	629	ILE	2.1
1	C	865	ALA	2.1
1	B	674	GLU	2.1
1	A	802	LYS	2.1
1	A	682	THR	2.0
1	A	775	THR	2.0
1	C	836	PRO	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 [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	TBR	B	1000	18/18	0.85	0.27	1.85	86,87,88,88	18
2	TBR	A	999	18/18	0.84	0.25	-0.05	83,86,87,88	18
2	TBR	C	1001	18/18	0.89	0.17	-3.41	86,87,88,89	18

### 6.5 Other polymers [i](#)

There are no such residues in this entry.