



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 01:13 PM EDT

PDB ID : 3AUZ  
Title : Crystal structure of Mre11 with manganese  
Authors : Park, Y.B.; Cho, Y.  
Deposited on : 2011-02-18  
Resolution : 3.21 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 types of validation reports are described at

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

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

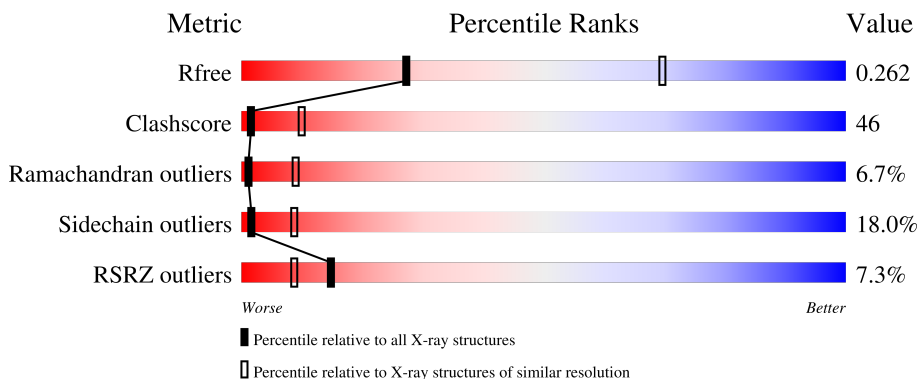
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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	333	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 2635 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 DNA double-strand break repair protein mre11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2627	1694	442	480	11	0	0	0

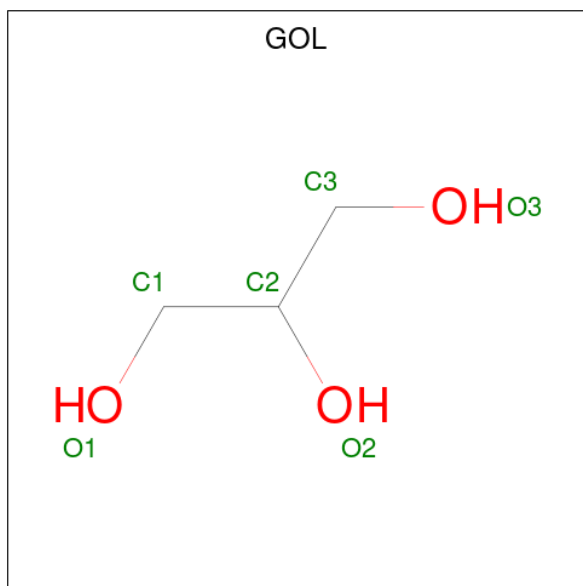
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q58719
A	-18	GLY	-	expression tag	UNP Q58719
A	-17	SER	-	expression tag	UNP Q58719
A	-16	SER	-	expression tag	UNP Q58719
A	-15	HIS	-	expression tag	UNP Q58719
A	-14	HIS	-	expression tag	UNP Q58719
A	-13	HIS	-	expression tag	UNP Q58719
A	-12	HIS	-	expression tag	UNP Q58719
A	-11	HIS	-	expression tag	UNP Q58719
A	-10	HIS	-	expression tag	UNP Q58719
A	-9	SER	-	expression tag	UNP Q58719
A	-8	SER	-	expression tag	UNP Q58719
A	-7	GLY	-	expression tag	UNP Q58719
A	-6	LEU	-	expression tag	UNP Q58719
A	-5	VAL	-	expression tag	UNP Q58719
A	-4	PRO	-	expression tag	UNP Q58719
A	-3	ARG	-	expression tag	UNP Q58719
A	-2	GLY	-	expression tag	UNP Q58719
A	-1	SER	-	expression tag	UNP Q58719
A	0	HIS	-	expression tag	UNP Q58719

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

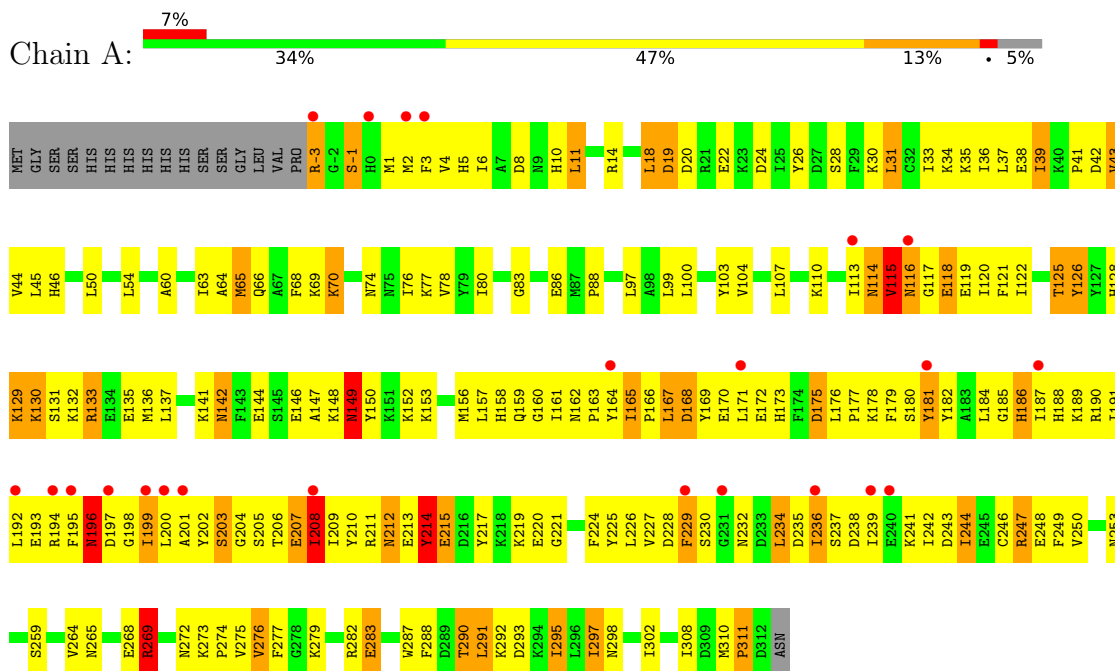


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

### 3 Residue-property plots

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: DNA double-strand break repair protein mre11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.98Å 101.98Å 113.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.05 – 3.21 49.43 – 3.21	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.05-3.21) 96.2 (49.43-3.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.219 , 0.263 0.221 , 0.262	Depositor DCC
$R_{free}$ test set	1025 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	92.4	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 73.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: GOL, MN

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	0.53	0/2684	0.70	0/3602

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	2627	0	2644	241	0
2	A	2	0	0	0	0
3	A	6	0	8	0	0
All	All	2635	0	2652	241	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 46.

All (241) 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:149:ASN:H	1:A:149:ASN:HD22	1.12	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LYS:CE	1:A:168:ASP:HB2	1.98	0.92
1:A:118:GLU:HG2	1:A:119:GLU:H	1.36	0.91
1:A:163:PRO:HG2	1:A:173:HIS:HB3	1.53	0.89
1:A:142:ASN:C	1:A:142:ASN:HD22	1.78	0.86
1:A:120:ILE:HG13	1:A:121:PHE:H	1.40	0.86
1:A:115:VAL:HG23	1:A:116:ASN:N	1.91	0.85
1:A:117:GLY:O	1:A:118:GLU:HB2	1.77	0.84
1:A:165:ILE:HD12	1:A:168:ASP:O	1.79	0.83
1:A:176:LEU:HD13	1:A:182:TYR:HE2	1.44	0.81
1:A:287:TRP:O	1:A:290:THR:HB	1.81	0.81
1:A:3:PHE:HB2	1:A:43:VAL:O	1.81	0.80
1:A:190:ARG:HD2	1:A:225:TYR:HE2	1.46	0.78
1:A:149:ASN:H	1:A:149:ASN:ND2	1.77	0.78
1:A:207:GLU:O	1:A:209:ILE:HG13	1.84	0.78
1:A:190:ARG:HD2	1:A:225:TYR:CE2	2.18	0.77
1:A:4:VAL:HG23	1:A:41:PRO:HG2	1.66	0.77
1:A:178:LYS:HG2	1:A:196:ASN:HB3	1.66	0.77
1:A:190:ARG:HB3	1:A:225:TYR:OH	1.85	0.77
1:A:190:ARG:HG3	1:A:221:GLY:O	1.84	0.77
1:A:165:ILE:HD13	1:A:165:ILE:O	1.87	0.75
1:A:181:TYR:CE2	1:A:227:VAL:HG21	2.22	0.74
1:A:44:VAL:HB	1:A:78:VAL:HG13	1.68	0.74
1:A:192:LEU:HB2	1:A:225:TYR:HE1	1.53	0.73
1:A:199:ILE:HD11	1:A:236:ILE:HG13	1.70	0.73
1:A:120:ILE:HD12	1:A:152:LYS:HB3	1.70	0.72
1:A:283:GLU:O	1:A:287:TRP:HZ3	1.73	0.72
1:A:208:ILE:HG22	1:A:210:TYR:O	1.91	0.71
1:A:2:MET:HA	1:A:228:ASP:HA	1.74	0.70
1:A:120:ILE:HG13	1:A:121:PHE:N	2.07	0.69
1:A:150:TYR:O	1:A:153:LYS:HE2	1.92	0.69
1:A:163:PRO:CG	1:A:173:HIS:HB3	2.20	0.68
1:A:288:PHE:O	1:A:291:LEU:HD12	1.94	0.68
1:A:30:LYS:HE3	1:A:63:ILE:HD13	1.75	0.68
1:A:132:LYS:HE3	1:A:135:GLU:HG2	1.77	0.67
1:A:283:GLU:O	1:A:287:TRP:CZ3	2.47	0.66
1:A:142:ASN:C	1:A:142:ASN:ND2	2.49	0.66
1:A:214:TYR:CG	1:A:215:GLU:N	2.65	0.65
1:A:149:ASN:HD22	1:A:149:ASN:N	1.93	0.64
1:A:182:TYR:HB2	1:A:200:LEU:HA	1.80	0.64
1:A:308:ILE:N	1:A:308:ILE:HD12	2.13	0.64
1:A:128:HIS:CG	1:A:136:MET:HE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LYS:O	1:A:189:LYS:HG3	1.98	0.63
1:A:130:LYS:HE3	1:A:168:ASP:HB2	1.80	0.63
1:A:172:GLU:O	1:A:175:ASP:HB2	1.98	0.63
1:A:165:ILE:O	1:A:165:ILE:HG23	2.00	0.62
1:A:264:VAL:HG22	1:A:291:LEU:HD21	1.80	0.61
1:A:181:TYR:HE2	1:A:227:VAL:HG21	1.64	0.61
1:A:1:MET:O	1:A:228:ASP:O	2.18	0.61
1:A:292:LYS:O	1:A:295:ILE:HG22	2.01	0.61
1:A:176:LEU:HD13	1:A:182:TYR:CE2	2.31	0.61
1:A:193:GLU:HG3	1:A:193:GLU:O	2.01	0.61
1:A:192:LEU:HD11	1:A:239:ILE:HD13	1.83	0.60
1:A:236:ILE:HD12	1:A:236:ILE:H	1.65	0.60
1:A:178:LYS:HA	1:A:182:TYR:OH	2.01	0.60
1:A:1:MET:SD	1:A:115:VAL:HG21	2.41	0.60
1:A:5:HIS:CE1	1:A:203:SER:H	2.19	0.60
1:A:4:VAL:HG11	1:A:36:ILE:HD11	1.83	0.60
1:A:54:LEU:HD21	1:A:88:PRO:HA	1.83	0.60
1:A:210:TYR:HB3	1:A:211:ARG:C	2.23	0.59
1:A:64:ALA:O	1:A:68:PHE:HD2	1.85	0.59
1:A:310:MET:HB3	1:A:311:PRO:CD	2.32	0.59
1:A:130:LYS:HE2	1:A:168:ASP:HB2	1.82	0.59
1:A:116:ASN:HD22	1:A:116:ASN:H	1.50	0.59
1:A:219:LYS:HG3	1:A:220:GLU:HG2	1.84	0.59
1:A:161:ILE:HG23	1:A:163:PRO:HD2	1.85	0.58
1:A:170:GLU:O	1:A:171:LEU:HD23	2.03	0.58
1:A:210:TYR:CB	1:A:211:ARG:HB2	2.32	0.58
1:A:200:LEU:C	1:A:200:LEU:HD23	2.23	0.58
1:A:159:GLN:HB3	1:A:170:GLU:OE1	2.04	0.57
1:A:43:VAL:HG23	1:A:77:LYS:HB3	1.86	0.57
1:A:210:TYR:HA	1:A:211:ARG:HB2	1.85	0.57
1:A:3:PHE:HA	1:A:41:PRO:HB3	1.87	0.57
1:A:114:ASN:O	1:A:115:VAL:HG22	2.04	0.57
1:A:14:ARG:HH12	1:A:19:ASP:CG	2.08	0.56
1:A:160:GLY:O	1:A:169:TYR:HB2	2.05	0.56
1:A:43:VAL:CG2	1:A:77:LYS:HB3	2.35	0.56
1:A:189:LYS:HE2	1:A:191:ILE:HG12	1.87	0.56
1:A:265:ASN:HB3	1:A:269:ARG:HH21	1.70	0.56
1:A:288:PHE:CE2	1:A:298:ASN:ND2	2.74	0.56
1:A:20:ASP:O	1:A:24:ASP:OD2	2.24	0.56
1:A:118:GLU:HG2	1:A:119:GLU:N	2.15	0.56
1:A:227:VAL:HG12	1:A:228:ASP:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:PHE:C	1:A:3:PHE:CD2	2.79	0.56
1:A:190:ARG:NE	1:A:221:GLY:O	2.38	0.56
1:A:116:ASN:N	1:A:116:ASN:HD22	2.04	0.55
1:A:4:VAL:HG23	1:A:41:PRO:CG	2.36	0.55
1:A:117:GLY:O	1:A:118:GLU:CB	2.54	0.55
1:A:187:ILE:HG22	1:A:189:LYS:HG2	1.87	0.55
1:A:210:TYR:CA	1:A:211:ARG:HB2	2.37	0.55
1:A:116:ASN:N	1:A:116:ASN:ND2	2.54	0.54
1:A:161:ILE:CG2	1:A:162:ASN:N	2.71	0.54
1:A:121:PHE:CE2	1:A:147:ALA:HB2	2.43	0.54
1:A:130:LYS:NZ	1:A:168:ASP:HB2	2.23	0.54
1:A:50:LEU:N	1:A:86:GLU:OE2	2.41	0.54
1:A:100:LEU:O	1:A:104:VAL:HB	2.08	0.54
1:A:161:ILE:CG2	1:A:163:PRO:HD2	2.37	0.54
1:A:115:VAL:CG2	1:A:116:ASN:N	2.64	0.54
1:A:214:TYR:O	1:A:217:TYR:HB3	2.08	0.54
1:A:235:ASP:C	1:A:237:SER:H	2.11	0.54
1:A:10:HIS:CD2	1:A:209:ILE:HD13	2.42	0.53
1:A:181:TYR:CE1	1:A:201:ALA:HB3	2.44	0.53
1:A:202:TYR:O	1:A:204:GLY:N	2.42	0.53
1:A:74:ASN:O	1:A:76:ILE:HG13	2.08	0.53
1:A:212:ASN:O	1:A:214:TYR:N	2.41	0.53
1:A:137:LEU:HD21	1:A:175:ASP:OD2	2.09	0.53
1:A:181:TYR:HE2	1:A:227:VAL:CG2	2.22	0.52
1:A:191:ILE:HB	1:A:202:TYR:HB2	1.91	0.52
1:A:202:TYR:O	1:A:203:SER:C	2.48	0.52
1:A:185:GLY:O	1:A:186:HIS:HB3	2.10	0.52
1:A:187:ILE:HG13	1:A:202:TYR:CZ	2.45	0.52
1:A:274:PRO:HD2	1:A:295:ILE:HA	1.92	0.52
1:A:83:GLY:HA2	1:A:158:HIS:CD2	2.45	0.52
1:A:224:PHE:CE2	1:A:242:ILE:HD13	2.45	0.52
1:A:120:ILE:CG1	1:A:121:PHE:N	2.73	0.52
1:A:210:TYR:CD1	1:A:211:ARG:HB2	2.45	0.52
1:A:276:VAL:CG1	1:A:295:ILE:HD11	2.40	0.51
1:A:210:TYR:HB3	1:A:211:ARG:HB2	1.91	0.51
1:A:210:TYR:HD1	1:A:211:ARG:HB2	1.76	0.51
1:A:-3:ARG:H1	1:A:-3:ARG:HH11	1.57	0.51
1:A:288:PHE:C	1:A:290:THR:N	2.61	0.51
1:A:180:SER:HB3	1:A:229:PHE:HZ	1.76	0.51
1:A:3:PHE:HB2	1:A:43:VAL:HG12	1.92	0.51
1:A:244:ILE:O	1:A:244:ILE:CG2	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:SER:HB2	1:A:2:MET:HG3	1.93	0.51
1:A:235:ASP:O	1:A:238:ASP:OD1	2.29	0.51
1:A:144:GLU:O	1:A:148:LYS:HG2	2.11	0.50
1:A:308:ILE:N	1:A:308:ILE:CD1	2.75	0.50
1:A:128:HIS:HB2	1:A:136:MET:CE	2.41	0.50
1:A:219:LYS:HG3	1:A:220:GLU:N	2.26	0.50
1:A:6:ILE:HA	1:A:203:SER:OG	2.11	0.50
1:A:162:ASN:ND2	1:A:169:TYR:CZ	2.79	0.50
1:A:165:ILE:HD13	1:A:165:ILE:C	2.32	0.50
1:A:220:GLU:HA	1:A:220:GLU:OE1	2.11	0.50
1:A:-3:ARG:H3	1:A:-3:ARG:HD2	1.77	0.50
1:A:176:LEU:HD12	1:A:176:LEU:O	2.10	0.50
1:A:288:PHE:HE2	1:A:298:ASN:ND2	2.09	0.50
1:A:-1:SER:HB3	1:A:230:SER:OG	2.12	0.50
1:A:39:ILE:HG21	1:A:226:LEU:HD22	1.94	0.50
1:A:310:MET:HB3	1:A:311:PRO:HD2	1.92	0.50
1:A:212:ASN:C	1:A:214:TYR:H	2.16	0.49
1:A:28:SER:HB3	1:A:207:GLU:HG3	1.93	0.49
1:A:187:ILE:CG1	1:A:202:TYR:CE1	2.95	0.49
1:A:209:ILE:O	1:A:209:ILE:HG22	2.12	0.49
1:A:3:PHE:HA	1:A:41:PRO:CB	2.43	0.49
1:A:268:GLU:OE2	1:A:268:GLU:HA	2.13	0.49
1:A:149:ASN:ND2	1:A:149:ASN:N	2.53	0.48
1:A:120:ILE:HD12	1:A:152:LYS:CB	2.41	0.48
1:A:2:MET:HG2	1:A:228:ASP:HB2	1.95	0.48
1:A:235:ASP:O	1:A:237:SER:N	2.47	0.48
1:A:97:LEU:C	1:A:99:LEU:H	2.17	0.48
1:A:282:ARG:NE	1:A:302:ILE:HG21	2.29	0.48
1:A:34:LYS:O	1:A:38:GLU:HG3	2.14	0.48
1:A:161:ILE:HG23	1:A:162:ASN:N	2.29	0.47
1:A:288:PHE:C	1:A:290:THR:H	2.17	0.47
1:A:3:PHE:CB	1:A:43:VAL:O	2.57	0.47
1:A:189:LYS:O	1:A:191:ILE:HG13	2.14	0.47
1:A:195:PHE:O	1:A:198:GLY:O	2.33	0.47
1:A:211:ARG:O	1:A:212:ASN:CB	2.62	0.47
1:A:132:LYS:CE	1:A:135:GLU:HG2	2.45	0.47
1:A:291:LEU:HD12	1:A:291:LEU:H	1.79	0.47
1:A:31:LEU:HD12	1:A:31:LEU:HA	1.73	0.47
1:A:185:GLY:O	1:A:186:HIS:CB	2.62	0.46
1:A:292:LYS:NZ	1:A:293:ASP:OD2	2.46	0.46
1:A:1:MET:SD	1:A:115:VAL:HG11	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HG11	1:A:36:ILE:CD1	2.45	0.46
1:A:2:MET:HG2	1:A:228:ASP:CB	2.46	0.46
1:A:141:LYS:HA	1:A:141:LYS:HD3	1.73	0.46
1:A:160:GLY:N	1:A:170:GLU:OE1	2.43	0.46
1:A:195:PHE:N	1:A:198:GLY:O	2.39	0.46
1:A:249:PHE:HA	1:A:275:VAL:O	2.16	0.46
1:A:39:ILE:HD13	1:A:226:LEU:HD22	1.98	0.45
1:A:165:ILE:O	1:A:165:ILE:CD1	2.62	0.45
1:A:187:ILE:HG13	1:A:202:TYR:CE1	2.51	0.45
1:A:188:HIS:CD2	1:A:205:SER:HB3	2.51	0.45
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.80	0.45
1:A:128:HIS:CG	1:A:136:MET:CE	3.00	0.45
1:A:46:HIS:HB3	1:A:80:ILE:HG13	1.98	0.45
1:A:163:PRO:HG2	1:A:173:HIS:CB	2.37	0.45
1:A:186:HIS:CD2	1:A:186:HIS:O	2.70	0.45
1:A:167:LEU:HA	1:A:168:ASP:HA	1.64	0.45
1:A:153:LYS:HG3	1:A:179:PHE:CD1	2.52	0.45
1:A:195:PHE:O	1:A:196:ASN:C	2.54	0.45
1:A:125:THR:HG23	1:A:126:TYR:N	2.32	0.45
1:A:275:VAL:HG22	1:A:297:ILE:HG22	1.99	0.45
1:A:125:THR:HG21	1:A:128:HIS:NE2	2.32	0.44
1:A:227:VAL:HG12	1:A:228:ASP:N	2.33	0.44
1:A:180:SER:CB	1:A:229:PHE:HZ	2.30	0.44
1:A:234:LEU:O	1:A:234:LEU:CD1	2.65	0.44
1:A:241:LYS:O	1:A:241:LYS:CG	2.65	0.44
1:A:2:MET:O	1:A:42:ASP:N	2.44	0.44
1:A:189:LYS:HD3	1:A:191:ILE:HD11	1.99	0.44
1:A:130:LYS:HZ1	1:A:168:ASP:HB2	1.82	0.44
1:A:114:ASN:HD22	1:A:114:ASN:HA	1.61	0.43
1:A:158:HIS:C	1:A:159:GLN:HG2	2.37	0.43
1:A:11:LEU:HB3	1:A:60:ALA:HB1	1.99	0.43
1:A:129:LYS:O	1:A:130:LYS:C	2.55	0.43
1:A:182:TYR:N	1:A:182:TYR:CD1	2.86	0.43
1:A:214:TYR:CD2	1:A:215:GLU:N	2.86	0.43
1:A:235:ASP:C	1:A:237:SER:N	2.70	0.43
1:A:142:ASN:HD21	1:A:146:GLU:CD	2.22	0.43
1:A:2:MET:HE2	1:A:226:LEU:HD11	2.01	0.43
1:A:200:LEU:HD23	1:A:201:ALA:N	2.33	0.43
1:A:249:PHE:HB3	1:A:277:PHE:HE2	1.83	0.43
1:A:253:ASN:O	1:A:259:SER:HB2	2.19	0.43
1:A:70:LYS:HA	1:A:70:LYS:HD2	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:MET:HE1	1:A:226:LEU:HD21	2.00	0.42
1:A:148:LYS:C	1:A:150:TYR:H	2.22	0.42
1:A:14:ARG:NH1	1:A:19:ASP:HA	2.35	0.42
1:A:161:ILE:HG23	1:A:162:ASN:H	1.83	0.42
1:A:164:TYR:CZ	1:A:200:LEU:HD13	2.55	0.42
1:A:164:TYR:OH	1:A:200:LEU:HD13	2.18	0.42
1:A:22:GLU:HG2	1:A:26:TYR:CE2	2.55	0.42
1:A:14:ARG:NH1	1:A:19:ASP:OD2	2.53	0.41
1:A:69:LYS:HA	1:A:103:TYR:CD2	2.55	0.41
1:A:214:TYR:CE2	1:A:215:GLU:HB3	2.55	0.41
1:A:136:MET:HE2	1:A:136:MET:HB2	1.97	0.41
1:A:161:ILE:HG22	1:A:164:TYR:HD2	1.85	0.41
1:A:65:MET:O	1:A:66:GLN:C	2.58	0.41
1:A:3:PHE:CD2	1:A:3:PHE:O	2.74	0.41
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.68	0.41
1:A:33:ILE:HD12	1:A:33:ILE:HG23	1.77	0.41
1:A:43:VAL:HG22	1:A:77:LYS:O	2.20	0.41
1:A:163:PRO:CD	1:A:173:HIS:HB3	2.51	0.41
1:A:167:LEU:HD12	1:A:168:ASP:N	2.36	0.41
1:A:190:ARG:NH1	1:A:224:PHE:O	2.54	0.41
1:A:234:LEU:O	1:A:234:LEU:HD13	2.21	0.41
1:A:128:HIS:HB2	1:A:136:MET:HE2	2.03	0.40
1:A:156:MET:O	1:A:157:LEU:HG	2.21	0.40
1:A:133:ARG:HH11	1:A:133:ARG:HG2	1.86	0.40
1:A:282:ARG:CZ	1:A:302:ILE:HG21	2.51	0.40
1:A:308:ILE:O	1:A:308:ILE:HG22	2.21	0.40
1:A:161:ILE:CG2	1:A:164:TYR:HD2	2.35	0.40
1:A:273:LYS:HA	1:A:274:PRO:HD3	1.95	0.40
1:A:11:LEU:HD12	1:A:11:LEU:HA	1.81	0.40
1:A:246:CYS:O	1:A:247:ARG:C	2.60	0.40
1:A:121:PHE:HE2	1:A:147:ALA:HB2	1.84	0.40
1:A:184:LEU:HD12	1:A:202:TYR:CZ	2.56	0.40
1:A:186:HIS:O	1:A:186:HIS:CG	2.75	0.40
1:A:190:ARG:CG	1:A:221:GLY:O	2.63	0.40
1:A:194:ARG:HB2	1:A:236:ILE:HD11	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	314/333 (94%)	255 (81%)	38 (12%)	21 (7%)	<b>1</b> <b>9</b>

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	VAL
1	A	118	GLU
1	A	212	ASN
1	A	126	TYR
1	A	196	ASN
1	A	203	SER
1	A	208	ILE
1	A	213	GLU
1	A	236	ILE
1	A	39	ILE
1	A	186	HIS
1	A	214	TYR
1	A	269	ARG
1	A	149	ASN
1	A	232	ASN
1	A	247	ARG
1	A	8	ASP
1	A	130	LYS
1	A	177	PRO
1	A	166	PRO
1	A	311	PRO

### 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	289/304 (95%)	237 (82%)	52 (18%)	1 9

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ARG
1	A	-1	SER
1	A	11	LEU
1	A	18	LEU
1	A	19	ASP
1	A	31	LEU
1	A	35	LYS
1	A	37	LEU
1	A	43	VAL
1	A	45	LEU
1	A	65	MET
1	A	70	LYS
1	A	110	LYS
1	A	113	ILE
1	A	114	ASN
1	A	115	VAL
1	A	116	ASN
1	A	122	ILE
1	A	125	THR
1	A	129	LYS
1	A	131	SER
1	A	133	ARG
1	A	142	ASN
1	A	149	ASN
1	A	165	ILE
1	A	167	LEU
1	A	168	ASP
1	A	175	ASP
1	A	181	TYR
1	A	196	ASN
1	A	197	ASP
1	A	199	ILE
1	A	206	THR
1	A	207	GLU
1	A	208	ILE

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Mol	Chain	Res	Type
1	A	214	TYR
1	A	215	GLU
1	A	229	PHE
1	A	234	LEU
1	A	243	ASP
1	A	244	ILE
1	A	248	GLU
1	A	250	VAL
1	A	269	ARG
1	A	272	ASN
1	A	276	VAL
1	A	279	LYS
1	A	283	GLU
1	A	290	THR
1	A	291	LEU
1	A	295	ILE
1	A	297	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	114	ASN
1	A	116	ASN
1	A	142	ASN
1	A	149	ASN
1	A	253	ASN
1	A	265	ASN
1	A	272	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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
3	GOL	A	411	-	5,5,5	0.39	0	5,5,5	0.86	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	A	411	-	-	0/4/4/4	-

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 [i](#)

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	316/333 (94%)	0.48	23 (7%) <b>15</b> <b>9</b>	54, 97, 150, 170	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	ILE	6.0
1	A	200	LEU	5.1
1	A	236	ILE	4.0
1	A	229	PHE	3.5
1	A	194	ARG	3.5
1	A	231	GLY	3.4
1	A	-3	ARG	3.2
1	A	239	ILE	3.1
1	A	181	TYR	3.1
1	A	116	ASN	3.0
1	A	192	LEU	3.0
1	A	164	TYR	3.0
1	A	195	PHE	2.9
1	A	0	HIS	2.9
1	A	171	LEU	2.9
1	A	201	ALA	2.7
1	A	208	ILE	2.5
1	A	197	ASP	2.4
1	A	113	ILE	2.2
1	A	3	PHE	2.1
1	A	187	ILE	2.1
1	A	240	GLU	2.1
1	A	2	MET	2.1

## 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 monosaccharides 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MN	A	402	1/1	0.64	0.11	122,122,122,122	0
2	MN	A	401	1/1	0.89	0.07	131,131,131,131	0
3	GOL	A	411	6/6	0.91	0.31	61,66,69,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.