



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:48 PM GMT

PDB ID : 1M6U  
Title : Crystal Structure of a Novel DNA-binding domain from Ndt80, a Transcriptional Activator Required for Meiosis in Yeast  
Authors : Montano, S.P.; Cote, M.L.; Fingerman, I.; Pierce, M.; Vershon, A.K.; Georgiadis, M.M.  
Deposited on : 2002-07-17  
Resolution : 2.30 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

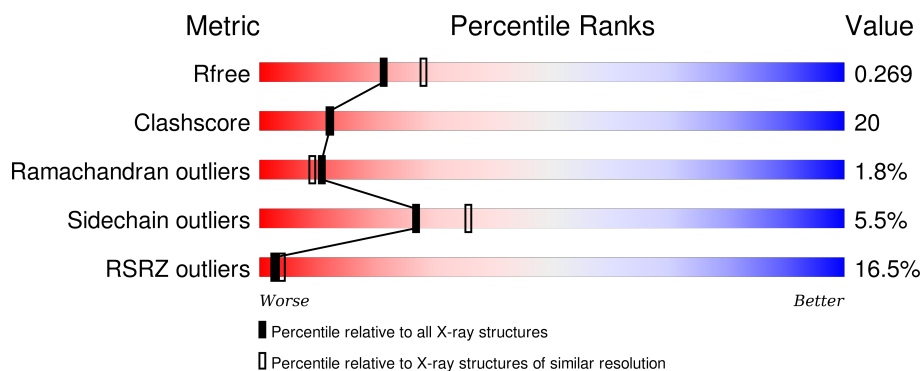
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	272	
1	B	272	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4187 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 Ndt80 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2109	1347	359	397	6			
1	B	250	Total	C	N	O	S	0	0	0
			1948	1249	329	364	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	THR	MET	SEE REMARK 999	UNP P38830
A	225	ASN	ASP	SEE REMARK 999	UNP P38830
A	267	PHE	SER	SEE REMARK 999	UNP P38830
B	213	THR	MET	SEE REMARK 999	UNP P38830
B	225	ASN	ASP	SEE REMARK 999	UNP P38830
B	267	PHE	SER	SEE REMARK 999	UNP P38830

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

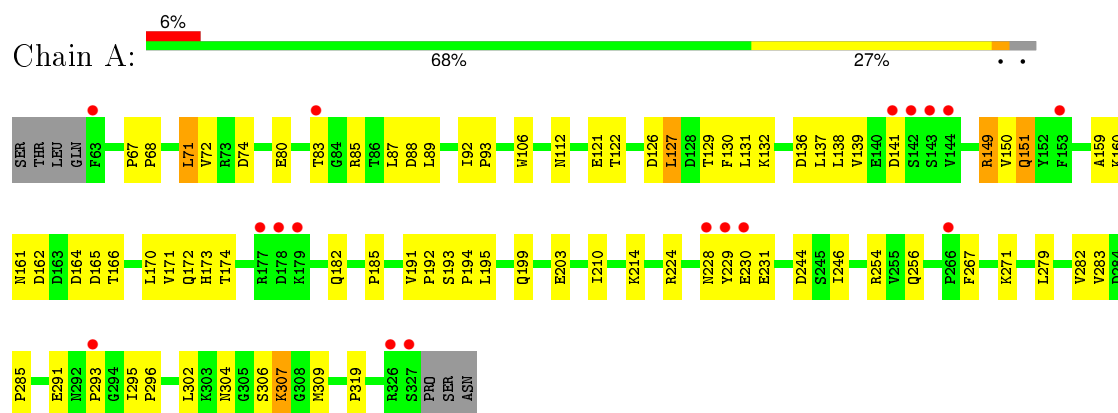
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	84	Total O 84 84	0	0
3	B	26	Total O 26 26	0	0

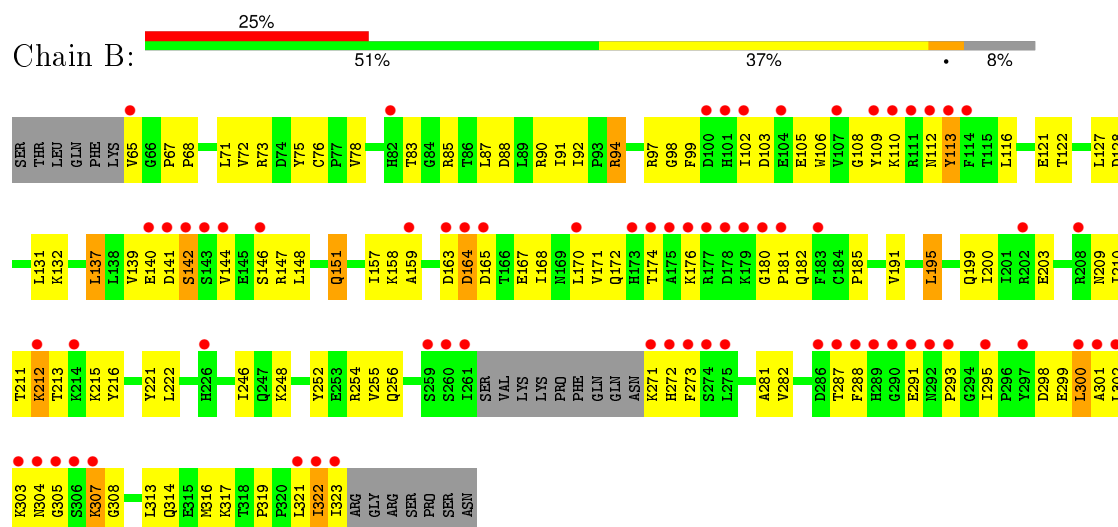
### 3 Residue-property plots [i](#)

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: Ndt80 protein



#### • Molecule 1: Ndt80 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.28Å 64.90Å 92.42Å 90.00° 107.52° 90.00°	Depositor
Resolution (Å)	19.96 – 2.30 19.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.7 (19.96-2.30) 95.3 (19.96-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.226 , 0.270 0.225 , 0.269	Depositor DCC
$R_{free}$ test set	1239 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 24433 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.39	0/2163	0.67	0/2942
1	B	0.34	0/1996	0.63	0/2720
All	All	0.37	0/4159	0.65	0/5662

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	2109	0	2027	61	0
1	B	1948	0	1854	100	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
3	A	84	0	0	1	0
3	B	26	0	0	2	0
All	All	4187	0	3881	159	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 20.

All (159) 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:200:ILE:HD12	1:B:200:ILE:H	1.33	0.91
1:B:172:GLN:HE21	1:B:185:PRO:HA	1.34	0.88
1:B:305:GLY:HA3	1:B:307:LYS:HE3	1.60	0.84
1:A:87:LEU:HD11	1:A:122:THR:HG22	1.63	0.78
1:B:209:ASN:HD21	1:B:212:LYS:HG2	1.47	0.78
1:A:307:LYS:HD2	1:A:307:LYS:H	1.49	0.78
1:B:68:PRO:O	1:B:319:PRO:HD3	1.83	0.77
1:B:172:GLN:NE2	1:B:185:PRO:HA	2.00	0.76
1:B:200:ILE:HD12	1:B:200:ILE:N	2.01	0.75
1:A:172:GLN:HE21	1:A:185:PRO:HA	1.52	0.75
1:B:172:GLN:HG2	1:B:255:VAL:HG22	1.70	0.74
1:B:109:TYR:HA	1:B:323:ILE:HG23	1.71	0.72
1:B:182:GLN:HA	1:B:182:GLN:HE21	1.55	0.71
1:B:301:ALA:C	1:B:302:LEU:HD12	2.11	0.71
1:A:228:ASN:O	1:A:231:GLU:HG2	1.90	0.70
1:B:302:LEU:HD11	1:B:308:GLY:HA3	1.72	0.70
1:A:164:ASP:O	1:A:166:THR:N	2.25	0.69
1:A:92:ILE:HD11	1:A:121:GLU:OE1	1.94	0.68
1:B:199:GLN:O	1:B:203:GLU:HB2	1.95	0.66
1:B:200:ILE:H	1:B:200:ILE:CD1	2.06	0.66
1:B:191:VAL:HG13	1:B:246:ILE:HG21	1.77	0.66
1:B:209:ASN:ND2	1:B:212:LYS:HG2	2.11	0.66
1:B:163:ASP:OD1	1:B:272:HIS:HB2	1.96	0.65
1:B:148:LEU:HD22	1:B:287:THR:CG2	2.26	0.65
1:B:302:LEU:HD12	1:B:302:LEU:N	2.12	0.65
1:B:151:GLN:HB2	1:B:282:VAL:O	1.97	0.65
1:A:173:HIS:NE2	1:A:256:GLN:NE2	2.45	0.64
1:A:68:PRO:O	1:A:319:PRO:HD3	1.98	0.64
1:B:72:VAL:HG22	1:B:317:LYS:HE3	1.80	0.63
1:A:307:LYS:HD2	1:A:307:LYS:N	2.11	0.62
1:B:148:LEU:HD22	1:B:287:THR:HG21	1.80	0.62
1:A:172:GLN:NE2	1:A:185:PRO:HA	2.14	0.62
1:B:113:TYR:HB3	1:B:254:ARG:HA	1.80	0.62
1:B:302:LEU:HD11	1:B:308:GLY:CA	2.31	0.61
1:A:191:VAL:HG13	1:A:246:ILE:HG21	1.83	0.60
1:A:68:PRO:HD2	1:A:319:PRO:HG2	1.83	0.60
1:B:83:THR:OG1	1:B:85:ARG:HG3	2.02	0.60
1:A:291:GLU:O	1:A:293:PRO:HD3	2.02	0.60
1:A:307:LYS:CD	1:A:307:LYS:H	2.15	0.59
1:A:302:LEU:HD12	1:A:306:SER:HB2	1.86	0.58
1:B:76:CYS:HB2	1:B:295:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:HG3	1:A:309:MET:CE	2.34	0.58
1:B:112:ASN:O	1:B:256:GLN:HB3	2.04	0.57
1:A:137:LEU:HD11	1:A:150:VAL:HG22	1.85	0.57
1:B:210:ILE:HD13	3:B:615:HOH:O	2.04	0.57
1:B:164:ASP:O	1:B:165:ASP:HB2	2.04	0.57
1:B:182:GLN:HA	1:B:182:GLN:NE2	2.19	0.57
1:B:157:ILE:HD13	1:B:252:TYR:CE1	2.40	0.57
1:B:91:ILE:H	1:B:314:GLN:NE2	2.03	0.57
1:A:136:ASP:OD1	1:A:149:ARG:HD3	2.05	0.57
1:B:211:THR:HG22	1:B:212:LYS:HE3	1.86	0.56
1:B:221:TYR:O	1:B:248:LYS:HE3	2.04	0.56
1:A:129:THR:CG2	1:B:180:GLY:HA2	2.35	0.56
1:B:323:ILE:HD12	1:B:323:ILE:N	2.20	0.56
1:B:322:ILE:HD13	1:B:322:ILE:N	2.21	0.56
1:B:159:ALA:HB2	1:B:170:LEU:HD21	1.88	0.55
1:B:90:ARG:HA	1:B:314:GLN:HE22	1.71	0.54
1:A:83:THR:HG22	1:A:85:ARG:HG3	1.88	0.54
1:B:300:LEU:N	1:B:300:LEU:HD13	2.23	0.54
1:B:302:LEU:HD11	1:B:308:GLY:N	2.22	0.54
1:B:112:ASN:HD22	1:B:113:TYR:N	2.05	0.53
1:B:112:ASN:ND2	1:B:113:TYR:N	2.56	0.53
1:B:73:ARG:HD3	1:B:75:TYR:OH	2.09	0.53
1:A:87:LEU:HD11	1:A:122:THR:CG2	2.34	0.53
1:A:88:ASP:O	1:A:122:THR:HA	2.08	0.53
1:A:224:ARG:HD2	1:A:244:ASP:OD1	2.08	0.53
1:B:94:ARG:O	1:B:116:LEU:HD12	2.09	0.53
1:B:210:ILE:HD12	1:B:210:ILE:N	2.24	0.53
1:B:99:PHE:CE2	1:B:321:LEU:HD13	2.44	0.53
1:B:213:THR:HG22	1:B:215:LYS:H	1.73	0.53
1:A:304:ASN:ND2	1:A:306:SER:OG	2.42	0.53
1:B:147:ARG:C	1:B:148:LEU:HD23	2.29	0.52
1:B:108:GLY:O	1:B:323:ILE:HA	2.09	0.52
1:B:271:LYS:N	1:B:271:LYS:HD2	2.24	0.52
1:A:224:ARG:HB3	1:A:244:ASP:HA	1.90	0.52
1:B:139:VAL:HB	1:B:146:SER:CB	2.40	0.52
1:A:295:ILE:HG23	1:A:296:PRO:HD2	1.90	0.52
1:A:83:THR:HG21	1:A:85:ARG:NE	2.25	0.50
1:B:73:ARG:HD3	1:B:75:TYR:CZ	2.46	0.50
1:B:121:GLU:HB2	3:B:612:HOH:O	2.11	0.50
1:A:171:VAL:CG1	1:A:182:GLN:HB3	2.41	0.50
1:B:140:GLU:OE1	1:B:140:GLU:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LYS:HB3	1:B:273:PHE:CE1	2.47	0.50
1:A:130:PHE:CE2	1:A:192:PRO:HD3	2.47	0.50
1:B:273:PHE:O	1:B:321:LEU:HB2	2.12	0.49
1:B:141:ASP:HB3	1:B:144:VAL:O	2.12	0.49
1:A:139:VAL:HG22	1:A:295:ILE:HD11	1.95	0.49
1:A:139:VAL:HG22	1:A:295:ILE:CD1	2.42	0.49
1:A:137:LEU:CD1	1:A:150:VAL:HG22	2.42	0.49
1:B:103:ASP:C	1:B:105:GLU:H	2.16	0.49
1:B:97:ARG:HG2	1:B:98:GLY:N	2.29	0.48
1:B:322:ILE:HD13	1:B:322:ILE:H	1.78	0.48
1:A:174:THR:O	1:A:254:ARG:NH1	2.46	0.48
1:B:158:LYS:NZ	1:B:298:ASP:OD1	2.42	0.48
1:B:112:ASN:HD22	1:B:113:TYR:H	1.62	0.48
1:B:271:LYS:HB3	1:B:273:PHE:HE1	1.78	0.47
1:A:161:ASN:HB3	1:A:164:ASP:O	2.14	0.47
1:B:71:LEU:HA	1:B:316:MET:HG2	1.96	0.47
1:A:112:ASN:HB3	3:A:702:HOH:O	2.14	0.47
1:B:210:ILE:HD12	1:B:210:ILE:H	1.79	0.47
1:A:151:GLN:HB2	1:A:282:VAL:O	2.15	0.46
1:B:88:ASP:O	1:B:122:THR:HA	2.16	0.46
1:B:108:GLY:O	1:B:323:ILE:HG23	2.16	0.46
1:B:72:VAL:HG22	1:B:317:LYS:HG2	1.98	0.46
1:B:131:LEU:HD11	1:B:222:LEU:HD21	1.99	0.45
1:B:281:ALA:HB2	1:B:313:LEU:HD11	1.98	0.45
1:A:159:ALA:HB2	1:A:170:LEU:HD21	1.98	0.45
1:B:147:ARG:O	1:B:148:LEU:HD23	2.17	0.44
1:B:291:GLU:C	1:B:293:PRO:HD3	2.38	0.44
1:A:87:LEU:HD13	1:A:88:ASP:N	2.32	0.44
1:B:174:THR:HA	1:B:254:ARG:HH11	1.81	0.44
1:B:167:GLU:HG2	1:B:168:ILE:N	2.32	0.44
1:B:172:GLN:HE21	1:B:185:PRO:CA	2.17	0.44
1:B:302:LEU:CD1	1:B:308:GLY:N	2.80	0.44
1:A:68:PRO:HD2	1:A:319:PRO:CG	2.47	0.44
1:B:168:ILE:HG13	1:B:273:PHE:CE2	2.53	0.44
1:A:80:GLU:HG3	1:B:181:PRO:CD	2.48	0.44
1:B:209:ASN:ND2	1:B:212:LYS:CG	2.79	0.44
1:B:128:ASP:OD1	1:B:132:LYS:HE3	2.18	0.44
1:A:203:GLU:OE2	1:A:210:ILE:HD13	2.18	0.43
1:A:229:TYR:O	1:A:231:GLU:N	2.52	0.43
1:A:87:LEU:HD13	1:A:87:LEU:C	2.38	0.43
1:A:267:PHE:O	1:A:271:LYS:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:HB3	1:A:160:LYS:HE2	1.77	0.43
1:A:132:LYS:HE2	1:A:231:GLU:HG3	2.00	0.43
1:B:65:VAL:O	1:B:106:TRP:CZ3	2.71	0.43
1:A:67:PRO:HG3	1:A:106:TRP:CE3	2.54	0.43
1:A:127:LEU:HD22	1:A:131:LEU:HD11	2.00	0.42
1:B:67:PRO:HA	1:B:68:PRO:HD3	1.79	0.42
1:A:71:LEU:HD23	1:A:72:VAL:N	2.33	0.42
1:A:149:ARG:HD3	1:A:149:ARG:HA	1.76	0.42
1:A:71:LEU:HD11	1:A:74:ASP:OD2	2.20	0.42
1:B:302:LEU:HB2	1:B:305:GLY:O	2.19	0.42
1:B:302:LEU:HD13	1:B:307:LYS:N	2.34	0.42
1:B:210:ILE:HG23	1:B:216:TYR:HB2	2.01	0.42
1:A:83:THR:O	1:A:83:THR:HG22	2.19	0.42
1:B:128:ASP:O	1:B:132:LYS:HG3	2.20	0.42
1:A:214:LYS:HB2	1:A:214:LYS:HE3	1.85	0.42
1:A:87:LEU:HD12	1:A:89:LEU:CD2	2.49	0.42
1:B:159:ALA:HB3	1:B:168:ILE:O	2.20	0.42
1:B:97:ARG:CG	1:B:98:GLY:N	2.83	0.42
1:A:83:THR:HG21	1:A:85:ARG:CD	2.50	0.42
1:B:171:VAL:HG13	1:B:182:GLN:HB2	2.02	0.41
1:A:283:VAL:HG23	1:A:309:MET:CE	2.50	0.41
1:B:182:GLN:NE2	1:B:182:GLN:CA	2.83	0.41
1:A:149:ARG:HB2	1:A:149:ARG:HH11	1.85	0.41
1:B:142:SER:C	1:B:144:VAL:H	2.23	0.41
1:B:302:LEU:N	1:B:302:LEU:CD1	2.81	0.41
1:A:193:SER:HA	1:A:194:PRO:HD3	1.91	0.41
1:B:72:VAL:CG2	1:B:317:LYS:HE3	2.50	0.41
1:B:92:ILE:HG22	1:B:195:LEU:HD12	2.02	0.41
1:A:138:LEU:HD12	1:A:138:LEU:HA	1.88	0.41
1:B:148:LEU:HD22	1:B:287:THR:HG22	2.00	0.40
1:B:210:ILE:CD1	1:B:210:ILE:H	2.34	0.40
1:A:87:LEU:HD12	1:A:89:LEU:HG	2.02	0.40
1:B:109:TYR:CD2	1:B:323:ILE:O	2.73	0.40
1:B:305:GLY:CA	1:B:307:LYS:HE3	2.40	0.40
1:B:78:VAL:HG22	1:B:137:LEU:HD12	2.02	0.40
1:A:126:ASP:OD2	1:A:126:ASP:N	2.55	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	263/272 (97%)	246 (94%)	14 (5%)	3 (1%)	17	18
1	B	246/272 (90%)	211 (86%)	29 (12%)	6 (2%)	7	5
All	All	509/544 (94%)	457 (90%)	43 (8%)	9 (2%)	11	9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ASP
1	A	162	ASP
1	A	230	GLU
1	B	110	LYS
1	B	303	LYS
1	B	176	LYS
1	B	102	ILE
1	B	142	SER
1	B	288	PHE

### 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	232/251 (92%)	222 (96%)	10 (4%)	35	47
1	B	208/251 (83%)	194 (93%)	14 (7%)	20	26
All	All	440/502 (88%)	416 (94%)	24 (6%)	27	36

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	93	PRO
1	A	127	LEU
1	A	141	ASP
1	A	149	ARG
1	A	151	GLN
1	A	195	LEU
1	A	199	GLN
1	A	279	LEU
1	A	307	LYS
1	B	87	LEU
1	B	94	ARG
1	B	113	TYR
1	B	127	LEU
1	B	137	LEU
1	B	151	GLN
1	B	164	ASP
1	B	195	LEU
1	B	212	LYS
1	B	299	GLU
1	B	300	LEU
1	B	304	ASN
1	B	307	LYS
1	B	322	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	172	GLN
1	A	182	GLN
1	A	199	GLN
1	A	256	GLN
1	B	172	GLN
1	B	182	GLN
1	B	206	ASN
1	B	209	ASN
1	B	226	HIS
1	B	228	ASN
1	B	256	GLN
1	B	304	ASN

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Mol	Chain	Res	Type
1	B	314	GLN

### 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 [i](#)

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	SO4	A	400	-	4,4,4	0.27	0	6,6,6	0.28	0
2	SO4	A	500	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	A	700	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	B	600	-	4,4,4	0.20	0	6,6,6	0.12	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
2	SO4	A	400	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	500	-	-	0/0/0/0	0/0/0/0
2	SO4	A	700	-	-	0/0/0/0	0/0/0/0
2	SO4	B	600	-	-	0/0/0/0	0/0/0/0

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 [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	265/272 (97%)	0.46	17 (6%) 23 31	17, 32, 62, 76	0
1	B	250/272 (91%)	1.47	68 (27%) 1 1	21, 50, 94, 104	0
All	All	515/544 (94%)	0.95	85 (16%) 2 4	17, 37, 88, 104	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	PHE	18.6
1	A	327	SER	10.3
1	B	289	HIS	9.3
1	B	290	GLY	7.6
1	B	142	SER	7.6
1	A	142	SER	7.5
1	B	175	ALA	7.4
1	B	143	SER	6.9
1	B	304	ASN	6.9
1	B	303	LYS	6.8
1	B	178	ASP	6.4
1	B	261	ILE	6.0
1	B	141	ASP	6.0
1	A	63	PHE	5.9
1	B	174	THR	5.8
1	B	177	ARG	5.6
1	B	176	LYS	5.5
1	B	163	ASP	5.5
1	B	144	VAL	5.2
1	B	165	ASP	4.8
1	B	260	SER	4.7
1	B	112	ASN	4.7
1	B	113	TYR	4.7
1	B	292	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	326	ARG	4.6
1	B	100	ASP	4.5
1	B	273	PHE	4.3
1	B	140	GLU	4.2
1	B	302	LEU	4.2
1	B	164	ASP	4.1
1	B	323	ILE	4.0
1	B	301	ALA	3.9
1	B	291	GLU	3.8
1	B	322	ILE	3.8
1	B	102	ILE	3.7
1	B	287	THR	3.7
1	B	306	SER	3.6
1	B	259	SER	3.6
1	B	272	HIS	3.6
1	A	229	TYR	3.6
1	B	109	TYR	3.6
1	A	143	SER	3.5
1	B	214	LYS	3.5
1	B	271	LYS	3.4
1	B	179	LYS	3.4
1	A	266	PRO	3.4
1	B	293	PRO	3.3
1	B	107	VAL	3.3
1	B	208	ARG	3.2
1	B	275	LEU	3.2
1	A	178	ASP	2.9
1	A	141	ASP	2.9
1	A	230	GLU	2.8
1	B	321	LEU	2.8
1	B	286	ASP	2.8
1	B	295	ILE	2.8
1	B	183	PHE	2.7
1	B	104	GLU	2.7
1	B	82	HIS	2.7
1	B	101	HIS	2.6
1	A	177	ARG	2.6
1	A	179	LYS	2.5
1	B	181	PRO	2.5
1	A	228	ASN	2.5
1	B	111	ARG	2.4
1	A	153	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	297	TYR	2.4
1	B	65	VAL	2.4
1	B	146	SER	2.4
1	B	212	LYS	2.4
1	A	144	VAL	2.3
1	B	110	LYS	2.3
1	B	274	SER	2.3
1	B	226	HIS	2.2
1	B	202	ARG	2.2
1	B	114	PHE	2.2
1	B	300	LEU	2.1
1	B	307	LYS	2.1
1	A	83	THR	2.1
1	A	293	PRO	2.1
1	B	305	GLY	2.1
1	B	159	ALA	2.1
1	B	170	LEU	2.1
1	B	173	HIS	2.1
1	B	180	GLY	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(Å <sup>2</sup> )	Q<0.9
2	SO4	A	500	5/5	0.94	0.16	0.29	65,66,67,67	0
2	SO4	A	400	5/5	0.98	0.13	-0.82	24,25,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	600	5/5	0.98	0.13	-1.13	49,50,51,52	0
2	SO4	A	700	5/5	0.99	0.08	-1.40	26,26,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.