



## Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:49 pm BST

PDB ID : 1VDZ  
Title : Crystal structure of A-type ATPase catalytic subunit A from *Pyrococcus horikoshii* OT3  
Authors : Maegawa, Y.; Morita, H.; Yao, M.; Watanabe, N.; Tanaka, I.  
Deposited on : 2004-03-26  
Resolution : 2.55 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.

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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 : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

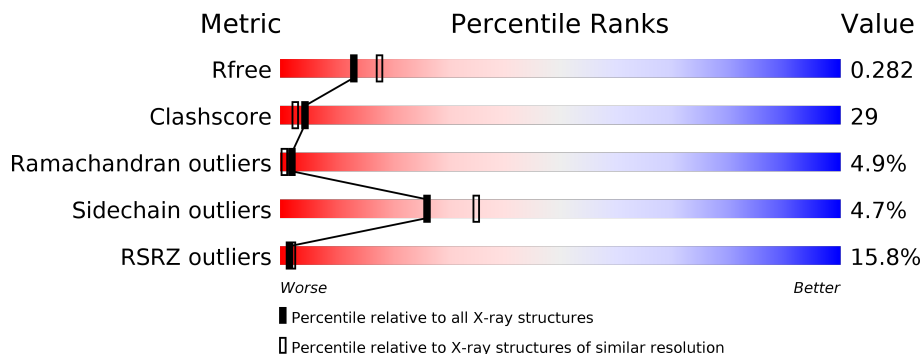
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	588	

## 2 Entry composition [i](#)

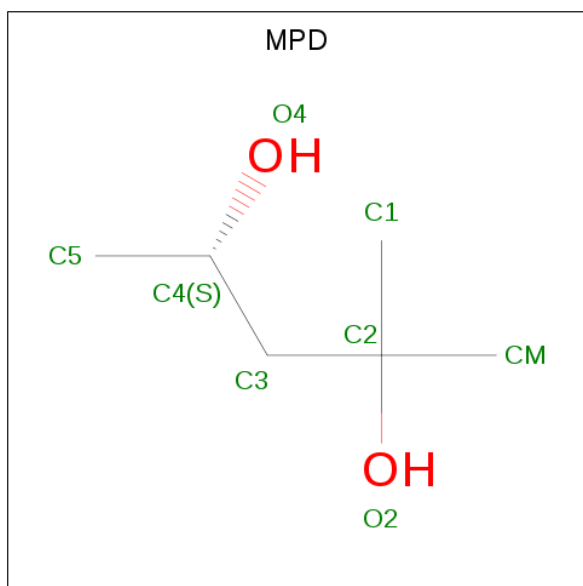
There are 2 unique types of molecules in this entry. The entry contains 4033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 A-type ATPase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	513	4025	2572	687	750	16	0	0	0

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).

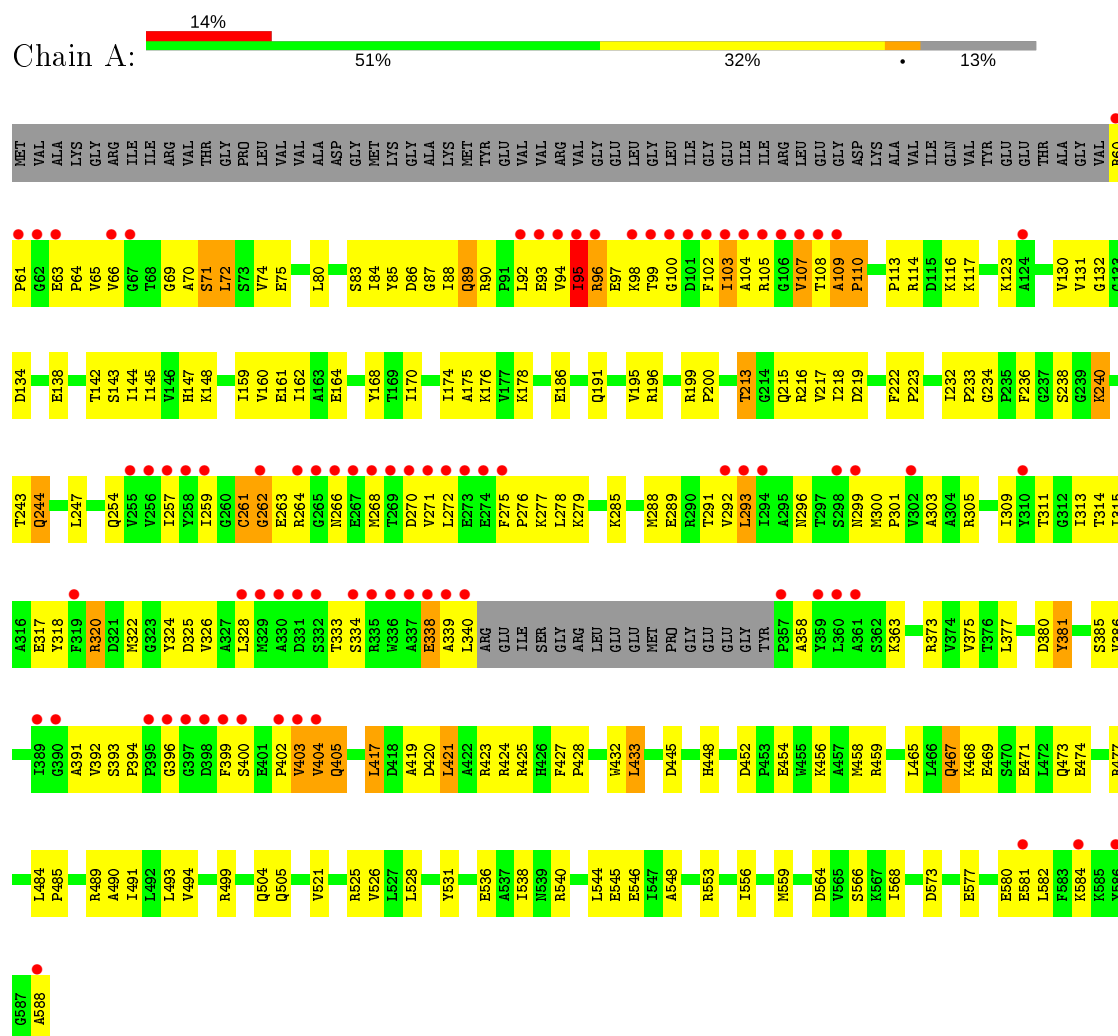


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	8	6	2	0	0

### 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 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: A-type ATPase subunit A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.98Å 127.98Å 104.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.55 38.63 – 2.55	Depositor EDS
% Data completeness (in resolution range)	92.1 (10.00-2.55) 99.9 (38.63-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.62 (at 2.54Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.239 , 0.271 0.250 , 0.282	Depositor DCC
$R_{free}$ test set	2923 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: MPD

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	0.36	0/4112	0.64	1/5566 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	VAL	N-CA-C	-5.34	96.58	111.00

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	4025	0	4058	233	0
2	A	8	0	14	0	0
All	All	4033	0	4072	233	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 29.

All (233) 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:191:GLN:NE2	1:A:199:ARG:HH22	1.43	1.17
1:A:333:THR:HG22	1:A:334:SER:H	1.21	1.05
1:A:97:GLU:HG2	1:A:98:LYS:H	1.18	1.04
1:A:103:ILE:HG22	1:A:104:ALA:H	1.19	1.04
1:A:261:CYS:HA	1:A:296:ASN:HB2	1.48	0.95
1:A:70:ALA:H	1:A:103:ILE:HG23	1.33	0.92
1:A:97:GLU:HG2	1:A:98:LYS:N	1.83	0.89
1:A:191:GLN:HE21	1:A:199:ARG:HH22	1.18	0.88
1:A:373:ARG:HG3	1:A:385:SER:HB3	1.53	0.88
1:A:213:THR:HG22	1:A:215:GLN:H	1.39	0.87
1:A:191:GLN:NE2	1:A:199:ARG:NH2	2.22	0.85
1:A:74:VAL:HG13	1:A:89:GLN:HE22	1.43	0.83
1:A:191:GLN:HE21	1:A:199:ARG:NH2	1.75	0.83
1:A:114:ARG:HD3	1:A:170:ILE:HD11	1.59	0.82
1:A:254:GLN:NE2	1:A:325:ASP:H	1.78	0.82
1:A:244:GLN:NE2	1:A:244:GLN:H	1.77	0.82
1:A:216:ARG:H	1:A:505:GLN:HE22	1.22	0.82
1:A:333:THR:HG22	1:A:334:SER:N	1.96	0.80
1:A:70:ALA:N	1:A:103:ILE:HG23	1.97	0.80
1:A:400:SER:O	1:A:405:GLN:HB2	1.82	0.79
1:A:213:THR:CG2	1:A:215:GLN:HG2	2.14	0.78
1:A:277:LYS:HE2	1:A:277:LYS:HA	1.66	0.77
1:A:103:ILE:HG22	1:A:104:ALA:N	1.97	0.77
1:A:546:GLU:HG3	1:A:582:LEU:HD11	1.66	0.76
1:A:72:LEU:HD12	1:A:72:LEU:H	1.50	0.76
1:A:96:ARG:HB3	1:A:301:PRO:HG2	1.65	0.75
1:A:99:THR:HG21	1:A:339:ALA:HB1	1.69	0.75
1:A:142:THR:HB	1:A:289:GLU:CG	2.18	0.74
1:A:458:MET:HE3	1:A:525:ARG:HG2	1.67	0.74
1:A:448:HIS:HE1	1:A:456:LYS:H	1.35	0.74
1:A:86:ASP:OD2	1:A:90:ARG:HG3	1.86	0.74
1:A:96:ARG:HH21	1:A:299:ASN:ND2	1.84	0.74
1:A:238:SER:OG	1:A:240:LYS:HG3	1.88	0.73
1:A:74:VAL:HG13	1:A:89:GLN:NE2	2.03	0.73
1:A:74:VAL:HG22	1:A:89:GLN:HE21	1.56	0.71
1:A:573:ASP:O	1:A:577:GLU:HG2	1.91	0.71
1:A:254:GLN:HE22	1:A:325:ASP:H	1.37	0.70
1:A:96:ARG:HG2	1:A:301:PRO:HD3	1.73	0.70
1:A:98:LYS:HB3	1:A:105:ARG:HG2	1.72	0.70
1:A:97:GLU:CG	1:A:98:LYS:H	2.02	0.69
1:A:404:VAL:HG13	1:A:405:GLN:H	1.56	0.69
1:A:98:LYS:HE2	1:A:105:ARG:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:H	1:A:505:GLN:NE2	1.92	0.67
1:A:419:ALA:O	1:A:423:ARG:HG3	1.95	0.66
1:A:559:MET:HG3	1:A:568:ILE:HG23	1.77	0.66
1:A:95:ILE:HD13	1:A:95:ILE:H	1.60	0.66
1:A:536:GLU:O	1:A:540:ARG:HG3	1.95	0.66
1:A:458:MET:CE	1:A:525:ARG:HG2	2.26	0.65
1:A:526:VAL:HG11	1:A:559:MET:HE2	1.78	0.65
1:A:191:GLN:HE22	1:A:199:ARG:HH22	1.43	0.64
1:A:144:ILE:HD12	1:A:289:GLU:HB3	1.79	0.64
1:A:233:PRO:HD2	1:A:417:LEU:HD22	1.79	0.64
1:A:403:VAL:HG23	1:A:404:VAL:H	1.62	0.63
1:A:271:VAL:HG13	1:A:275:PHE:CD1	2.33	0.63
1:A:142:THR:HB	1:A:289:GLU:HG3	1.79	0.63
1:A:404:VAL:HG13	1:A:405:GLN:N	2.14	0.63
1:A:499:ARG:O	1:A:504:GLN:HG3	1.98	0.63
1:A:96:ARG:CG	1:A:301:PRO:HD3	2.28	0.63
1:A:261:CYS:O	1:A:263:GLU:HG3	1.99	0.63
1:A:244:GLN:HE21	1:A:244:GLN:H	1.48	0.62
1:A:427:PHE:HA	1:A:428:PRO:C	2.19	0.62
1:A:148:LYS:HB2	1:A:322:MET:HG2	1.82	0.61
1:A:317:GLU:O	1:A:320:ARG:HG3	2.01	0.61
1:A:262:GLY:HA3	1:A:333:THR:OG1	2.00	0.61
1:A:340:LEU:HD23	1:A:363:LYS:HD3	1.83	0.61
1:A:448:HIS:CE1	1:A:456:LYS:H	2.18	0.60
1:A:70:ALA:O	1:A:71:SER:HB2	2.00	0.60
1:A:490:ALA:HB2	1:A:538:ILE:CD1	2.32	0.60
1:A:123:LYS:HE3	1:A:138:GLU:OE1	2.02	0.60
1:A:95:ILE:C	1:A:96:ARG:HD2	2.21	0.60
1:A:425:ARG:HH11	1:A:425:ARG:HG3	1.67	0.59
1:A:261:CYS:SG	1:A:262:GLY:N	2.74	0.59
1:A:526:VAL:HG11	1:A:559:MET:CE	2.33	0.59
1:A:162:ILE:HD12	1:A:174:ILE:O	2.03	0.58
1:A:394:PRO:HG2	1:A:399:PHE:CG	2.37	0.58
1:A:485:PRO:O	1:A:489:ARG:HG3	2.03	0.58
1:A:196:ARG:HH11	1:A:196:ARG:HG3	1.68	0.58
1:A:74:VAL:HG22	1:A:89:GLN:NE2	2.17	0.58
1:A:114:ARG:CD	1:A:170:ILE:HD11	2.32	0.58
1:A:311:THR:O	1:A:315:ILE:HG13	2.02	0.58
1:A:85:TYR:HB3	1:A:89:GLN:HA	1.85	0.58
1:A:94:VAL:HG22	1:A:95:ILE:N	2.19	0.58
1:A:216:ARG:N	1:A:505:GLN:HE22	1.99	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:PRO:HG2	1:A:399:PHE:CD1	2.39	0.57
1:A:176:LYS:HE2	1:A:186:GLU:HG2	1.86	0.57
1:A:257:ILE:HB	1:A:328:LEU:HD12	1.86	0.57
1:A:213:THR:HG23	1:A:215:GLN:HG2	1.87	0.56
1:A:161:GLU:OE1	1:A:176:LYS:HD2	2.05	0.56
1:A:88:ILE:HD13	1:A:97:GLU:HB2	1.86	0.56
1:A:90:ARG:HD2	1:A:94:VAL:HG11	1.88	0.56
1:A:263:GLU:OE1	1:A:268:MET:HA	2.06	0.56
1:A:400:SER:HA	1:A:405:GLN:NE2	2.21	0.56
1:A:259:ILE:HD13	1:A:309:ILE:HA	1.87	0.56
1:A:467:GLN:O	1:A:471:GLU:HG3	2.05	0.56
1:A:95:ILE:HG13	1:A:107:VAL:CG1	2.36	0.56
1:A:95:ILE:HG13	1:A:107:VAL:HB	1.87	0.56
1:A:142:THR:HB	1:A:289:GLU:HG2	1.88	0.55
1:A:213:THR:HB	1:A:219:ASP:OD1	2.05	0.55
1:A:70:ALA:HB2	1:A:103:ILE:CG2	2.36	0.55
1:A:232:ILE:HD11	1:A:417:LEU:HD21	1.89	0.55
1:A:102:PHE:CD1	1:A:103:ILE:N	2.73	0.55
1:A:545:GLU:H	1:A:545:GLU:CD	2.09	0.55
1:A:490:ALA:HB2	1:A:538:ILE:HD12	1.88	0.55
1:A:333:THR:CG2	1:A:334:SER:H	2.00	0.55
1:A:259:ILE:CD1	1:A:309:ILE:HA	2.37	0.55
1:A:143:SER:OG	1:A:285:LYS:HD3	2.07	0.54
1:A:94:VAL:HG22	1:A:95:ILE:HG12	1.89	0.54
1:A:95:ILE:CD1	1:A:95:ILE:H	2.17	0.54
1:A:130:VAL:HG11	1:A:159:ILE:HD11	1.88	0.54
1:A:268:MET:HE3	1:A:272:LEU:HB2	1.90	0.54
1:A:454:GLU:O	1:A:458:MET:HG3	2.07	0.54
1:A:108:THR:O	1:A:109:ALA:CB	2.56	0.54
1:A:100:GLY:HA3	1:A:102:PHE:CE2	2.44	0.53
1:A:277:LYS:CE	1:A:277:LYS:HA	2.37	0.53
1:A:556:ILE:HA	1:A:559:MET:HE3	1.89	0.53
1:A:232:ILE:HG12	1:A:417:LEU:CD2	2.38	0.53
1:A:99:THR:HG23	1:A:100:GLY:N	2.23	0.53
1:A:261:CYS:HB2	1:A:296:ASN:HD22	1.74	0.53
1:A:577:GLU:O	1:A:580:GLU:HB2	2.08	0.53
1:A:291:THR:HG22	1:A:292:VAL:N	2.24	0.53
1:A:556:ILE:HG23	1:A:559:MET:HE1	1.90	0.53
1:A:94:VAL:HG22	1:A:95:ILE:H	1.74	0.52
1:A:469:GLU:O	1:A:473:GLN:HG3	2.09	0.52
1:A:458:MET:HE1	1:A:525:ARG:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLU:OE2	1:A:588:ALA:HA	2.09	0.52
1:A:320:ARG:HG2	1:A:386:VAL:HG23	1.92	0.52
1:A:581:GLU:OE1	1:A:584:LYS:HD2	2.10	0.51
1:A:213:THR:HG22	1:A:215:GLN:HG2	1.89	0.51
1:A:275:PHE:C	1:A:277:LYS:H	2.14	0.51
1:A:147:HIS:HE1	1:A:318:TYR:OH	1.93	0.51
1:A:278:LEU:HD13	1:A:279:LYS:N	2.27	0.50
1:A:108:THR:O	1:A:109:ALA:HB2	2.11	0.50
1:A:468:LYS:HD2	1:A:491:ILE:HD13	1.93	0.50
1:A:96:ARG:HB3	1:A:301:PRO:CG	2.39	0.50
1:A:213:THR:HG22	1:A:215:GLN:N	2.18	0.50
1:A:458:MET:CE	1:A:528:LEU:HD12	2.42	0.50
1:A:380:ASP:O	1:A:381:TYR:HB3	2.12	0.49
1:A:546:GLU:CG	1:A:582:LEU:HD11	2.38	0.49
1:A:90:ARG:CD	1:A:94:VAL:HG11	2.42	0.49
1:A:313:ILE:O	1:A:317:GLU:HG3	2.13	0.49
1:A:99:THR:HB	1:A:303:ALA:HB1	1.95	0.49
1:A:75:GLU:OE1	1:A:114:ARG:NH2	2.46	0.48
1:A:333:THR:CG2	1:A:334:SER:N	2.67	0.48
1:A:75:GLU:H	1:A:89:GLN:HE22	1.62	0.48
1:A:131:VAL:HG22	1:A:134:ASP:OD2	2.14	0.48
1:A:95:ILE:HG21	1:A:107:VAL:HG11	1.95	0.48
1:A:160:VAL:HG11	1:A:178:LYS:HE3	1.96	0.48
1:A:275:PHE:O	1:A:277:LYS:N	2.47	0.48
1:A:521:VAL:O	1:A:525:ARG:HG3	2.14	0.47
1:A:162:ILE:HD12	1:A:175:ALA:HB2	1.96	0.47
1:A:70:ALA:O	1:A:71:SER:CB	2.62	0.47
1:A:420:ASP:O	1:A:424:ARG:HD3	2.14	0.47
1:A:96:ARG:NH2	1:A:299:ASN:ND2	2.59	0.47
1:A:277:LYS:CA	1:A:277:LYS:HE2	2.40	0.47
1:A:548:ALA:O	1:A:553:ARG:NH1	2.46	0.47
1:A:264:ARG:NH1	1:A:264:ARG:HG2	2.30	0.46
1:A:99:THR:HB	1:A:303:ALA:CB	2.45	0.46
1:A:232:ILE:CD1	1:A:417:LEU:HD21	2.45	0.46
1:A:80:LEU:O	1:A:83:SER:HB3	2.15	0.46
1:A:399:PHE:C	1:A:404:VAL:HG11	2.36	0.46
1:A:84:ILE:CG2	1:A:92:LEU:HD22	2.45	0.46
1:A:103:ILE:CG2	1:A:104:ALA:N	2.69	0.45
1:A:275:PHE:C	1:A:277:LYS:N	2.69	0.45
1:A:392:VAL:CG1	1:A:404:VAL:HB	2.46	0.45
1:A:264:ARG:HG2	1:A:264:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:CG1	1:A:89:GLN:HE22	2.22	0.45
1:A:448:HIS:HA	1:A:452:ASP:O	2.17	0.45
1:A:458:MET:SD	1:A:525:ARG:HG2	2.56	0.45
1:A:69:GLY:H	1:A:103:ILE:HG12	1.81	0.45
1:A:394:PRO:CG	1:A:399:PHE:HA	2.47	0.45
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.81	0.45
1:A:313:ILE:HD12	1:A:328:LEU:HD22	1.98	0.44
1:A:100:GLY:C	1:A:102:PHE:H	2.21	0.44
1:A:489:ARG:HB2	1:A:544:LEU:HD22	1.98	0.44
1:A:232:ILE:HG12	1:A:417:LEU:HD21	1.99	0.44
1:A:243:THR:O	1:A:247:LEU:HG	2.16	0.44
1:A:317:GLU:HA	1:A:320:ARG:HG2	2.00	0.44
1:A:458:MET:CE	1:A:525:ARG:HA	2.48	0.44
1:A:96:ARG:NH1	1:A:300:MET:HG2	2.33	0.44
1:A:452:ASP:OD2	1:A:525:ARG:NH1	2.46	0.44
1:A:60:ARG:N	1:A:107:VAL:O	2.50	0.44
1:A:393:SER:C	1:A:403:VAL:HG21	2.38	0.44
1:A:261:CYS:O	1:A:262:GLY:C	2.57	0.43
1:A:114:ARG:HD3	1:A:170:ILE:CD1	2.40	0.43
1:A:95:ILE:HB	1:A:107:VAL:HG21	2.00	0.43
1:A:84:ILE:HG21	1:A:92:LEU:HD22	2.00	0.43
1:A:113:PRO:HB2	1:A:116:LYS:HB2	2.01	0.43
1:A:164:GLU:O	1:A:168:TYR:OH	2.30	0.43
1:A:392:VAL:HG11	1:A:404:VAL:HB	2.00	0.43
1:A:427:PHE:O	1:A:504:GLN:HA	2.19	0.43
1:A:195:VAL:HA	1:A:314:THR:OG1	2.19	0.43
1:A:215:GLN:HA	1:A:505:GLN:HE22	1.84	0.42
1:A:95:ILE:HG13	1:A:107:VAL:CB	2.48	0.42
1:A:421:LEU:HA	1:A:421:LEU:HD12	1.88	0.42
1:A:144:ILE:HG22	1:A:145:ILE:CD1	2.49	0.42
1:A:232:ILE:O	1:A:391:ALA:HA	2.19	0.42
1:A:109:ALA:HA	1:A:110:PRO:HD3	1.88	0.42
1:A:432:TRP:CD1	1:A:433:LEU:HD13	2.55	0.42
1:A:320:ARG:HA	1:A:324:TYR:O	2.19	0.42
1:A:474:GLU:O	1:A:477:ARG:HB3	2.20	0.42
1:A:564:ASP:OD1	1:A:566:SER:OG	2.34	0.42
1:A:92:LEU:O	1:A:93:GLU:HB2	2.20	0.42
1:A:380:ASP:O	1:A:381:TYR:CB	2.68	0.42
1:A:236:PHE:CE2	1:A:391:ALA:HB2	2.54	0.42
1:A:148:LYS:HB2	1:A:322:MET:CG	2.50	0.41
1:A:232:ILE:CG1	1:A:417:LEU:HD21	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLU:OE2	1:A:525:ARG:NH2	2.53	0.41
1:A:116:LYS:HD3	1:A:117:LYS:N	2.35	0.41
1:A:288:MET:HE1	1:A:291:THR:HG21	2.02	0.41
1:A:92:LEU:HD12	1:A:93:GLU:H	1.84	0.41
1:A:132:GLY:O	1:A:377:LEU:HB3	2.21	0.41
1:A:199:ARG:HA	1:A:200:PRO:HD3	1.84	0.41
1:A:95:ILE:N	1:A:95:ILE:HD13	2.31	0.41
1:A:217:VAL:HG13	1:A:218:ILE:N	2.35	0.41
1:A:238:SER:OG	1:A:240:LYS:CG	2.64	0.41
1:A:288:MET:HE1	1:A:293:LEU:HD23	2.03	0.41
1:A:338:GLU:O	1:A:338:GLU:HG3	2.21	0.41
1:A:399:PHE:CA	1:A:404:VAL:HG11	2.51	0.41
1:A:262:GLY:CA	1:A:333:THR:OG1	2.68	0.41
1:A:425:ARG:NH1	1:A:425:ARG:HG3	2.33	0.41
1:A:494:VAL:HG11	1:A:531:TYR:HB2	2.03	0.41
1:A:559:MET:HB2	1:A:559:MET:HE3	1.91	0.41
1:A:244:GLN:HE21	1:A:244:GLN:N	2.17	0.41
1:A:296:ASN:OD1	1:A:305:ARG:HA	2.21	0.41
1:A:577:GLU:H	1:A:577:GLU:HG2	1.68	0.41
1:A:222:PHE:N	1:A:223:PRO:HD3	2.36	0.41
1:A:400:SER:O	1:A:404:VAL:HG13	2.21	0.41
1:A:490:ALA:HB2	1:A:538:ILE:HD11	2.03	0.41
1:A:90:ARG:HH22	1:A:96:ARG:HA	1.85	0.40
1:A:90:ARG:NH2	1:A:96:ARG:HA	2.36	0.40
1:A:99:THR:OG1	1:A:100:GLY:N	2.49	0.40
1:A:96:ARG:HD2	1:A:96:ARG:N	2.36	0.40
1:A:399:PHE:HA	1:A:404:VAL:HG11	2.03	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	509/588 (87%)	439 (86%)	45 (9%)	25 (5%)	2 1

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	PRO
1	A	63	GLU
1	A	64	PRO
1	A	71	SER
1	A	89	GLN
1	A	109	ALA
1	A	266	ASN
1	A	358	ALA
1	A	402	PRO
1	A	403	VAL
1	A	65	VAL
1	A	66	VAL
1	A	87	GLY
1	A	95	ILE
1	A	107	VAL
1	A	234	GLY
1	A	262	GLY
1	A	338	GLU
1	A	103	ILE
1	A	261	CYS
1	A	110	PRO
1	A	381	TYR
1	A	404	VAL
1	A	396	GLY
1	A	276	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	428/492 (87%)	408 (95%)	20 (5%)	26 35

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	95	ILE
1	A	96	ARG
1	A	213	THR
1	A	240	LYS
1	A	244	GLN
1	A	270	ASP
1	A	293	LEU
1	A	320	ARG
1	A	326	VAL
1	A	405	GLN
1	A	417	LEU
1	A	421	LEU
1	A	433	LEU
1	A	445	ASP
1	A	459	ARG
1	A	465	LEU
1	A	467	GLN
1	A	484	LEU
1	A	493	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	147	HIS
1	A	191	GLN
1	A	244	GLN
1	A	245	HIS
1	A	254	GLN
1	A	405	GLN
1	A	426	HIS
1	A	448	HIS
1	A	467	GLN
1	A	504	GLN
1	A	505	GLN
1	A	539	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	MPD	A	589	-	7,7,7	0.56	0	9,10,10	0.48	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	MPD	A	589	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	589	MPD	O2-C2-C3-C4

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	513/588 (87%)	0.83	81 (15%) <b>2</b>   <b>2</b>	25, 49, 101, 101	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	19.6
1	A	107	VAL	13.9
1	A	339	ALA	13.3
1	A	268	MET	10.0
1	A	95	ILE	9.6
1	A	61	PRO	9.5
1	A	357	PRO	7.9
1	A	108	THR	7.8
1	A	272	LEU	7.5
1	A	337	ALA	7.2
1	A	62	GLY	7.0
1	A	96	ARG	6.9
1	A	101	ASP	6.8
1	A	264	ARG	6.8
1	A	60	ARG	6.7
1	A	588	ALA	6.5
1	A	404	VAL	6.1
1	A	336	TRP	5.7
1	A	98	LYS	5.6
1	A	338	GLU	5.0
1	A	398	ASP	4.8
1	A	92	LEU	4.7
1	A	94	VAL	4.6
1	A	273	GLU	4.6
1	A	403	VAL	4.5
1	A	99	THR	4.3
1	A	63	GLU	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	265	GLY	4.2
1	A	102	PHE	4.2
1	A	302	VAL	4.0
1	A	359	TYR	4.0
1	A	262	GLY	4.0
1	A	402	PRO	3.9
1	A	257	ILE	3.9
1	A	269	THR	3.8
1	A	266	ASN	3.8
1	A	103	ILE	3.6
1	A	298	SER	3.4
1	A	100	GLY	3.4
1	A	395	PRO	3.4
1	A	360	LEU	3.3
1	A	389	ILE	3.2
1	A	400	SER	3.2
1	A	584	LYS	3.1
1	A	256	VAL	3.1
1	A	328	LEU	3.1
1	A	270	ASP	3.0
1	A	361	ALA	3.0
1	A	106	GLY	3.0
1	A	329	MET	2.8
1	A	109	ALA	2.8
1	A	255	VAL	2.7
1	A	66	VAL	2.7
1	A	396	GLY	2.7
1	A	67	GLY	2.7
1	A	258	TYR	2.7
1	A	274	GLU	2.6
1	A	294	ILE	2.6
1	A	292	VAL	2.6
1	A	581	GLU	2.6
1	A	104	ALA	2.5
1	A	390	GLY	2.5
1	A	310	TYR	2.5
1	A	293	LEU	2.5
1	A	397	GLY	2.4
1	A	319	PHE	2.4
1	A	399	PHE	2.4
1	A	331	ASP	2.3
1	A	275	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	335	ARG	2.2
1	A	332	SER	2.2
1	A	334	SER	2.2
1	A	330	ALA	2.2
1	A	299	ASN	2.2
1	A	105	ARG	2.2
1	A	93	GLU	2.2
1	A	586	TYR	2.1
1	A	124	ALA	2.1
1	A	271	VAL	2.1
1	A	267	GLU	2.1
1	A	259	ILE	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MPD	A	589	8/8	0.89	0.39	85,85,86,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.