



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:51 AM GMT

PDB ID : 3ND9  
Title : Structural characterization for the nucleotide binding ability of subunit A of the A1AO ATP synthase  
Authors : Kumar, A.; Jeyakanthan, J.; Gruber, G.  
Deposited on : 2010-06-07  
Resolution : 3.10 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

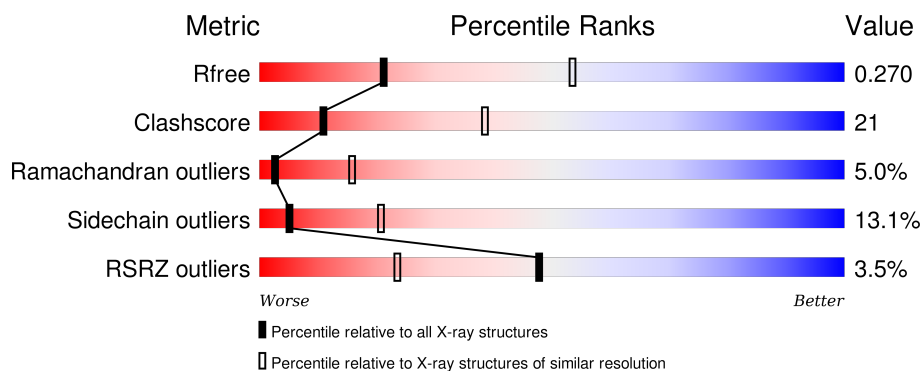
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	588	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MRD	A	590	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4047 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.

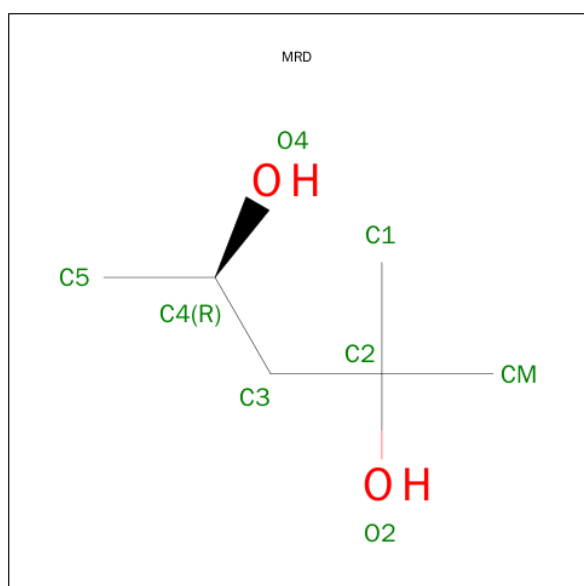
- Molecule 1 is a protein called V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	508	4004	2560	685	743	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ARG	GLY	ENGINEERED MUTATION	UNP O57728
A	241	ALA	THR	ENGINEERED MUTATION	UNP O57728

- Molecule 2 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



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

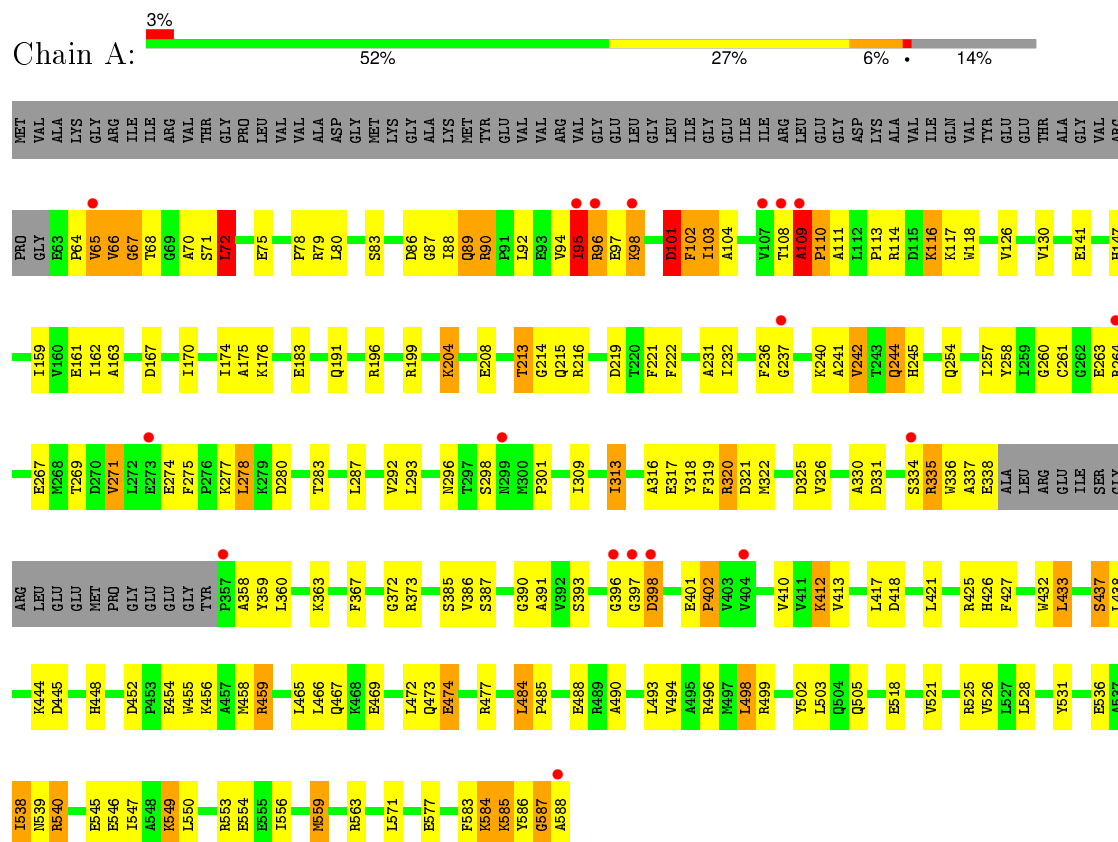
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		

### 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: V-type ATP synthase alpha chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.38 Å 128.38 Å 105.06 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.10 29.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.90-3.10) 100.0 (29.90-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 3.11 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.220 , 0.285 0.215 , 0.270	Depositor DCC
$R_{free}$ test set	834 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 16465 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4047	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: MRD

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	0.75	1/4091 (0.0%)	0.84	6/5539 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	PRO	N-CD	10.35	1.62	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ALA	CB-CA-C	10.65	126.08	110.10
1	A	109	ALA	C-N-CD	-7.90	103.23	120.60
1	A	417	LEU	CA-CB-CG	6.23	129.62	115.30
1	A	110	PRO	N-CA-C	-5.31	98.29	112.10
1	A	110	PRO	N-CA-CB	5.19	109.53	103.30
1	A	110	PRO	CA-N-CD	-5.14	104.31	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	GLY	Peptide
1	A	95	ILE	Peptide

## 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	4004	0	4046	169	0
2	A	16	0	28	3	0
3	A	27	0	0	2	0
All	All	4047	0	4074	170	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 21.

All (170) 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:97:GLU:HG2	1:A:98:LYS:H	1.18	1.08
1:A:70:ALA:H	1:A:103:ILE:HG23	1.28	0.96
1:A:75:GLU:H	1:A:89:GLN:HE22	1.11	0.94
1:A:103:ILE:HG22	1:A:104:ALA:H	1.37	0.90
1:A:584:LYS:HG2	1:A:585:LYS:N	1.91	0.85
1:A:261:CYS:HA	1:A:296:ASN:HB2	1.59	0.84
1:A:216:ARG:H	1:A:505:GLN:HE22	1.20	0.84
1:A:496:ARG:HA	1:A:499:ARG:NH1	1.92	0.84
1:A:556:ILE:HA	1:A:559:MET:HE3	1.58	0.83
1:A:426:HIS:HE1	3:A:614:HOH:O	1.61	0.82
1:A:97:GLU:HG2	1:A:98:LYS:N	1.92	0.82
1:A:162:ILE:HD12	1:A:175:ALA:HB2	1.63	0.81
1:A:70:ALA:N	1:A:103:ILE:HG23	1.97	0.80
1:A:72:LEU:H	1:A:72:LEU:HD12	1.47	0.80
1:A:213:THR:HG22	1:A:215:GLN:H	1.47	0.78
1:A:68:THR:CG2	1:A:101:ASP:O	2.30	0.78
1:A:70:ALA:HB2	1:A:103:ILE:HG21	1.66	0.78
1:A:103:ILE:HG22	1:A:104:ALA:N	1.98	0.77
1:A:213:THR:HB	1:A:219:ASP:OD1	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:LYS:CG	1:A:585:LYS:N	2.49	0.75
1:A:540:ARG:NH2	1:A:583:PHE:HB3	2.02	0.74
1:A:448:HIS:HE1	1:A:456:LYS:H	1.35	0.74
1:A:191:GLN:NE2	1:A:199:ARG:HH22	1.85	0.74
1:A:147:HIS:HE1	1:A:318:TYR:OH	1.71	0.74
1:A:108:THR:O	1:A:109:ALA:CB	2.36	0.73
1:A:86:ASP:OD2	1:A:90:ARG:HG3	1.88	0.73
1:A:191:GLN:NE2	1:A:199:ARG:NH2	2.36	0.73
1:A:584:LYS:HG2	1:A:585:LYS:H	1.53	0.72
1:A:401:GLU:HG3	1:A:402:PRO:HA	1.72	0.71
1:A:587:GLY:O	1:A:588:ALA:HB3	1.90	0.71
1:A:108:THR:O	1:A:109:ALA:HB2	1.91	0.71
1:A:401:GLU:CG	1:A:402:PRO:HA	2.21	0.70
1:A:75:GLU:OE1	1:A:114:ARG:NH2	2.24	0.70
1:A:261:CYS:HB3	1:A:331:ASP:HB3	1.73	0.70
1:A:261:CYS:HB3	1:A:331:ASP:O	1.92	0.69
1:A:373:ARG:HG3	1:A:385:SER:HB3	1.75	0.68
1:A:526:VAL:HG11	1:A:559:MET:CE	2.23	0.68
1:A:271:VAL:HA	1:A:275:PHE:HD1	1.56	0.68
1:A:585:LYS:HG3	1:A:585:LYS:O	1.93	0.67
1:A:585:LYS:O	1:A:585:LYS:CG	2.43	0.66
1:A:79:ARG:HG2	1:A:118:TRP:HZ2	1.61	0.66
1:A:526:VAL:HG11	1:A:559:MET:HE2	1.76	0.66
1:A:584:LYS:O	1:A:587:GLY:N	2.29	0.65
1:A:584:LYS:O	1:A:586:TYR:N	2.30	0.65
1:A:98:LYS:HE2	1:A:98:LYS:O	1.97	0.64
1:A:587:GLY:O	1:A:588:ALA:CB	2.45	0.63
1:A:518:GLU:CD	1:A:518:GLU:H	2.02	0.62
1:A:242:VAL:HA	1:A:244:GLN:OE1	2.00	0.62
1:A:103:ILE:CG2	1:A:104:ALA:H	2.02	0.62
1:A:490:ALA:HB2	1:A:538:ILE:HD12	1.82	0.61
1:A:213:THR:CG2	1:A:215:GLN:H	2.13	0.61
1:A:254:GLN:NE2	1:A:325:ASP:H	1.99	0.59
1:A:469:GLU:O	1:A:473:GLN:HG3	2.03	0.58
1:A:216:ARG:H	1:A:505:GLN:NE2	1.96	0.58
1:A:216:ARG:N	1:A:505:GLN:HE22	1.97	0.58
1:A:79:ARG:HG2	1:A:118:TRP:CZ2	2.38	0.57
1:A:521:VAL:O	1:A:525:ARG:HG3	2.05	0.56
1:A:199:ARG:NH1	1:A:321:ASP:OD2	2.39	0.56
1:A:90:ARG:HB3	1:A:109:ALA:HB1	1.88	0.56
1:A:80:LEU:O	1:A:83:SER:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ILE:HG23	1:A:559:MET:HE1	1.87	0.55
1:A:75:GLU:H	1:A:89:GLN:NE2	1.91	0.55
1:A:432:TRP:CD1	1:A:433:LEU:HD13	2.42	0.55
1:A:130:VAL:HG11	1:A:159:ILE:HD11	1.89	0.54
1:A:147:HIS:CE1	1:A:318:TYR:OH	2.57	0.54
1:A:236:PHE:CZ	1:A:391:ALA:HB2	2.43	0.54
1:A:75:GLU:N	1:A:89:GLN:HE22	1.92	0.53
1:A:70:ALA:N	1:A:103:ILE:CG2	2.70	0.53
1:A:413:VAL:HG13	1:A:437:SER:HB2	1.91	0.52
1:A:536:GLU:O	1:A:540:ARG:HG3	2.10	0.52
1:A:90:ARG:HB3	1:A:109:ALA:CB	2.39	0.52
1:A:494:VAL:HG11	1:A:531:TYR:HB2	1.92	0.52
1:A:231:ALA:HA	1:A:390:GLY:O	2.10	0.52
1:A:244:GLN:HG2	1:A:245:HIS:N	2.25	0.51
1:A:401:GLU:CD	1:A:402:PRO:HA	2.31	0.51
1:A:275:PHE:HA	1:A:278:LEU:HD23	1.92	0.51
1:A:433:LEU:CD2	2:A:589:MRD:H1C3	2.41	0.51
1:A:412:LYS:HG3	1:A:438:LEU:HD12	1.93	0.51
1:A:257:ILE:HD12	1:A:292:VAL:HB	1.91	0.51
1:A:191:GLN:HE22	1:A:199:ARG:HH22	1.57	0.51
1:A:540:ARG:HH22	1:A:583:PHE:HB3	1.74	0.51
1:A:68:THR:HG22	1:A:101:ASP:O	2.10	0.51
1:A:264:ARG:H	1:A:267:GLU:HB3	1.76	0.51
1:A:213:THR:HG23	1:A:215:GLN:HG2	1.93	0.50
1:A:97:GLU:H	1:A:301:PRO:HG2	1.77	0.50
1:A:586:TYR:O	1:A:587:GLY:O	2.30	0.50
1:A:64:PRO:O	1:A:65:VAL:O	2.30	0.49
1:A:221:PHE:O	1:A:459:ARG:NH2	2.36	0.49
1:A:458:MET:CE	1:A:525:ARG:HG2	2.42	0.49
1:A:103:ILE:CG2	1:A:104:ALA:N	2.65	0.49
1:A:396:GLY:C	1:A:398:ASP:H	2.16	0.49
1:A:585:LYS:HG2	1:A:586:TYR:CE1	2.48	0.49
1:A:585:LYS:HG2	1:A:586:TYR:CD1	2.48	0.49
1:A:448:HIS:HA	1:A:452:ASP:O	2.13	0.49
1:A:583:PHE:O	1:A:587:GLY:N	2.46	0.49
1:A:214:GLY:N	1:A:219:ASP:OD2	2.46	0.49
2:A:589:MRD:H5C3	2:A:589:MRD:HMC2	1.94	0.49
1:A:458:MET:HE1	1:A:525:ARG:HG2	1.94	0.48
1:A:335:ARG:HB3	1:A:337:ALA:O	2.13	0.48
1:A:546:GLU:OE2	1:A:585:LYS:HE2	2.13	0.48
1:A:244:GLN:HG2	1:A:245:HIS:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ALA:HB3	1:A:360:LEU:HD12	1.95	0.48
1:A:96:ARG:HD2	1:A:96:ARG:N	2.29	0.48
1:A:78:PRO:O	1:A:79:ARG:HB2	2.14	0.48
1:A:334:SER:O	1:A:335:ARG:HB2	2.13	0.48
1:A:68:THR:HG21	1:A:101:ASP:O	2.12	0.48
1:A:241:ALA:O	1:A:244:GLN:OE1	2.32	0.47
1:A:317:GLU:HG2	1:A:320:ARG:NH1	2.29	0.47
1:A:88:ILE:HD11	1:A:90:ARG:CZ	2.44	0.47
1:A:191:GLN:HE21	1:A:199:ARG:NH2	2.11	0.47
1:A:72:LEU:CD1	1:A:72:LEU:H	2.23	0.47
1:A:222:PHE:HA	1:A:437:SER:HB3	1.97	0.47
1:A:584:LYS:C	1:A:586:TYR:N	2.68	0.46
1:A:113:PRO:HB2	1:A:116:LYS:HB2	1.97	0.46
1:A:452:ASP:OD2	1:A:525:ARG:NH1	2.48	0.46
1:A:141:GLU:OE1	1:A:147:HIS:HD2	1.99	0.46
1:A:213:THR:HG22	1:A:215:GLN:N	2.23	0.46
1:A:396:GLY:O	1:A:398:ASP:N	2.49	0.46
1:A:236:PHE:HB3	1:A:258:TYR:OH	2.16	0.45
1:A:66:VAL:O	1:A:67:GLY:O	2.35	0.45
1:A:448:HIS:CE1	1:A:456:LYS:H	2.25	0.45
1:A:232:ILE:O	1:A:391:ALA:HA	2.17	0.45
1:A:264:ARG:N	1:A:267:GLU:HB3	2.32	0.45
1:A:472:LEU:CD1	1:A:488:GLU:HG3	2.47	0.45
1:A:114:ARG:HD3	1:A:170:ILE:HD11	1.97	0.44
1:A:241:ALA:C	1:A:244:GLN:HE22	2.21	0.44
1:A:174:ILE:HG13	1:A:174:ILE:H	1.66	0.44
1:A:547:ILE:O	1:A:550:LEU:HB2	2.18	0.44
1:A:216:ARG:HB3	1:A:502:TYR:CE2	2.52	0.44
1:A:94:VAL:HG22	1:A:95:ILE:H	1.82	0.44
1:A:444:LYS:HA	1:A:455:TRP:CZ3	2.53	0.44
1:A:553:ARG:HB3	1:A:553:ARG:HE	1.63	0.44
1:A:545:GLU:O	1:A:549:LYS:HG2	2.18	0.44
1:A:401:GLU:HG3	1:A:402:PRO:CA	2.44	0.44
1:A:584:LYS:C	1:A:586:TYR:H	2.20	0.43
1:A:425:ARG:HA	1:A:427:PHE:CE1	2.53	0.43
1:A:216:ARG:NH2	1:A:505:GLN:HG3	2.33	0.43
1:A:433:LEU:HD23	2:A:589:MRD:H1C3	2.00	0.43
1:A:313:ILE:O	1:A:316:ALA:HB3	2.18	0.43
1:A:98:LYS:HE2	1:A:98:LYS:C	2.37	0.43
1:A:320:ARG:HG2	1:A:386:VAL:HG23	2.01	0.43
1:A:236:PHE:CE1	1:A:330:ALA:O	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ARG:HA	1:A:499:ARG:HH12	1.80	0.43
1:A:528:LEU:O	1:A:531:TYR:HB3	2.18	0.43
1:A:70:ALA:CB	1:A:103:ILE:HG21	2.44	0.43
1:A:559:MET:HE2	1:A:571:LEU:HD12	2.01	0.43
1:A:309:ILE:HB	1:A:367:PHE:CE1	2.54	0.43
1:A:418:ASP:OD1	1:A:418:ASP:C	2.57	0.43
1:A:75:GLU:CD	1:A:114:ARG:HH22	2.21	0.42
1:A:319:PHE:HA	1:A:322:MET:HE3	2.01	0.42
1:A:161:GLU:OE1	1:A:176:LYS:HD2	2.19	0.42
1:A:363:LYS:HE3	1:A:363:LYS:HB3	1.91	0.42
1:A:490:ALA:HB2	1:A:538:ILE:CD1	2.48	0.42
1:A:97:GLU:CG	1:A:98:LYS:N	2.71	0.42
1:A:325:ASP:OD1	1:A:385:SER:OG	2.34	0.42
1:A:278:LEU:HD13	1:A:278:LEU:HA	1.82	0.41
1:A:70:ALA:HB2	1:A:103:ILE:CG2	2.44	0.41
1:A:426:HIS:CE1	3:A:614:HOH:O	2.50	0.41
1:A:526:VAL:HG11	1:A:559:MET:HE1	1.98	0.41
1:A:556:ILE:O	1:A:559:MET:HB2	2.21	0.41
1:A:466:LEU:HG	1:A:498:LEU:HD12	2.02	0.41
1:A:254:GLN:HE22	1:A:325:ASP:H	1.65	0.41
1:A:484:LEU:HA	1:A:485:PRO:HD3	1.88	0.41
1:A:280:ASP:HB2	1:A:287:LEU:HA	2.03	0.41
1:A:204:LYS:HD2	1:A:372:GLY:HA3	2.02	0.40
1:A:469:GLU:OE1	1:A:499:ARG:HD3	2.22	0.40
1:A:236:PHE:HE1	1:A:330:ALA:O	2.05	0.40
1:A:126:VAL:HG23	1:A:162:ILE:HG22	2.03	0.40
1:A:79:ARG:HA	1:A:79:ARG:HD2	1.87	0.40
1:A:474:GLU:O	1:A:477:ARG:HB2	2.21	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	504/588 (86%)	443 (88%)	36 (7%)	25 (5%)	3	16

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	71	SER
1	A	89	GLN
1	A	101	ASP
1	A	109	ALA
1	A	110	PRO
1	A	67	GLY
1	A	87	GLY
1	A	102	PHE
1	A	397	GLY
1	A	559	MET
1	A	585	LYS
1	A	587	GLY
1	A	72	LEU
1	A	163	ALA
1	A	103	ILE
1	A	111	ALA
1	A	263	GLU
1	A	335	ARG
1	A	402	PRO
1	A	66	VAL
1	A	208	GLU
1	A	242	VAL
1	A	271	VAL
1	A	237	GLY

### 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	427/492 (87%)	371 (87%)	56 (13%)	5	21

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	90	ARG
1	A	92	LEU
1	A	95	ILE
1	A	96	ARG
1	A	98	LYS
1	A	101	ASP
1	A	102	PHE
1	A	116	LYS
1	A	117	LYS
1	A	167	ASP
1	A	183	GLU
1	A	196	ARG
1	A	204	LYS
1	A	213	THR
1	A	240	LYS
1	A	244	GLN
1	A	269	THR
1	A	274	GLU
1	A	277	LYS
1	A	278	LEU
1	A	283	THR
1	A	293	LEU
1	A	298	SER
1	A	313	ILE
1	A	320	ARG
1	A	326	VAL
1	A	336	TRP
1	A	338	GLU
1	A	359	TYR
1	A	387	SER
1	A	393	SER
1	A	398	ASP
1	A	410	VAL
1	A	412	LYS
1	A	421	LEU
1	A	433	LEU
1	A	437	SER
1	A	445	ASP
1	A	454	GLU
1	A	459	ARG
1	A	465	LEU

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Mol	Chain	Res	Type
1	A	467	GLN
1	A	474	GLU
1	A	484	LEU
1	A	493	LEU
1	A	498	LEU
1	A	503	LEU
1	A	538	ILE
1	A	539	ASN
1	A	540	ARG
1	A	549	LYS
1	A	554	GLU
1	A	563	ARG
1	A	577	GLU
1	A	584	LYS

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	89	GLN
1	A	147	HIS
1	A	191	GLN
1	A	244	GLN
1	A	254	GLN
1	A	405	GLN
1	A	426	HIS
1	A	448	HIS
1	A	467	GLN
1	A	505	GLN
1	A	539	ASN

### 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

2 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	MRD	A	589	-	6,7,7	0.33	0	7,10,10	0.50	0
2	MRD	A	590	-	6,7,7	0.45	0	7,10,10	0.44	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	MRD	A	589	-	-	0/5/5/5	0/0/0/0
2	MRD	A	590	-	-	0/5/5/5	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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	589	MRD	3	0



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	508/588 (86%)	-0.23	18 (3%)	48 23	29, 57, 120, 133	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	ILE	7.7
1	A	108	THR	5.7
1	A	107	VAL	5.5
1	A	109	ALA	5.3
1	A	96	ARG	4.9
1	A	397	GLY	3.5
1	A	273	GLU	3.2
1	A	404	VAL	3.1
1	A	396	GLY	2.9
1	A	357	PRO	2.7
1	A	65	VAL	2.7
1	A	398	ASP	2.5
1	A	237	GLY	2.5
1	A	299	ASN	2.4
1	A	264	ARG	2.2
1	A	588	ALA	2.2
1	A	98	LYS	2.2
1	A	334	SER	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MRD	A	590	8/8	0.76	0.40	8.59	87,90,91,92	0
2	MRD	A	589	8/8	0.93	0.21	1.26	79,80,81,82	0

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

There are no such residues in this entry.