



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:38 AM GMT

PDB ID : 3MFY
Title : Structural characterization of the subunit A mutant F236A of the A-ATP synthase from *Pyrococcus horikoshii*
Authors : Balakrishna, A.M.; Kumar, A.; Manimekali, M.S.S.; Jeyakanthan, J.; Gruber, G.
Deposited on : 2010-04-05
Resolution : 2.35 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

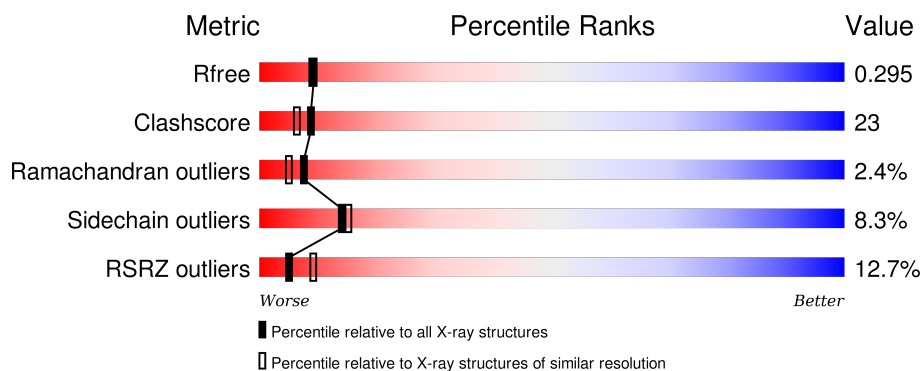
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 ≥ 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	MPD	A	589	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	A	590	-	-	-	X
2	MPD	A	592	-	-	-	X
2	MPD	A	593	-	-	X	X
3	TRS	A	591	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4356 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.

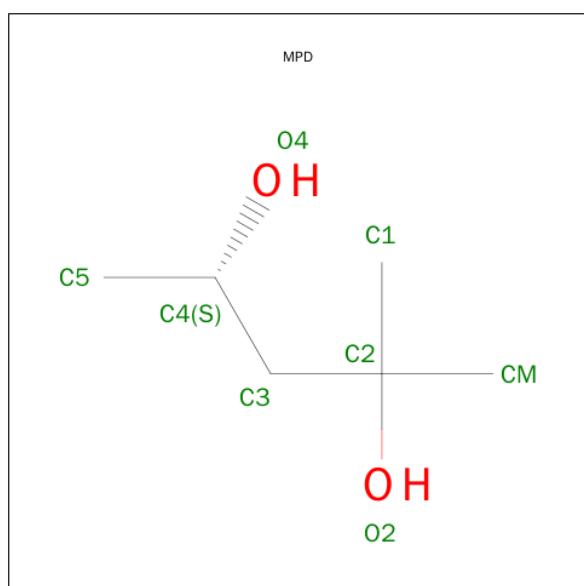
- Molecule 1 is a protein called V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	512	4039	2583	689	751	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	236	ALA	PHE	ENGINEERED MUTATION	UNP O57728

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



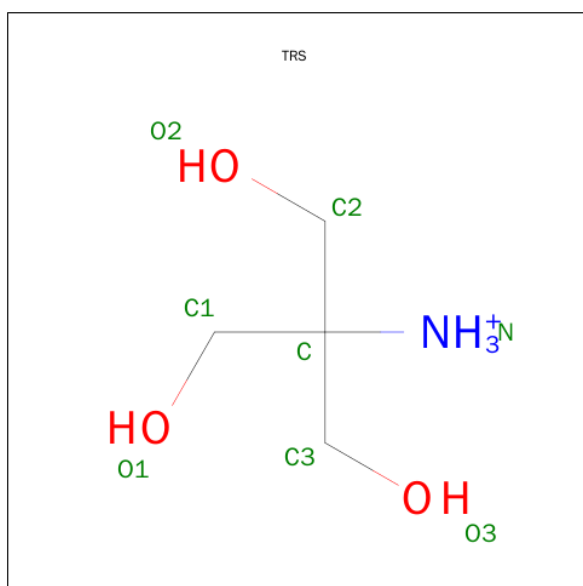
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		

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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		
2	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	265	Total	O	0	0
			265	265		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.53Å 127.53Å 106.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.75 – 2.35 19.75 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.75-2.35) 99.7 (19.75-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.222 , 0.279 0.243 , 0.295	Depositor DCC
R_{free} test set	1850 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 37138 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4356	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ACY, MPD, TRS

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	0.81	0/4127	0.81	7/5591 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	433	LEU	CB-CG-CD1	5.76	120.79	111.00
1	A	553	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	320	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	484	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	421	LEU	CB-CG-CD1	5.20	119.85	111.00
1	A	320	ARG	CG-CD-NE	-5.18	100.91	111.80
1	A	290	ARG	NE-CZ-NH1	-5.16	117.72	120.30

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	4039	0	4099	188	0
2	A	40	0	62	34	0
3	A	8	0	12	0	0
4	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	265	0	0	22	3
All	All	4356	0	4176	194	3

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 23.

All (194) 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:433:LEU:HD22	2:A:593:MPD:C5	1.53	1.38
1:A:433:LEU:CD2	2:A:593:MPD:C5	2.02	1.38
1:A:95:ILE:CG2	1:A:301:PRO:HD2	1.67	1.22
1:A:191:GLN:NE2	1:A:199:ARG:HH22	1.37	1.21
1:A:433:LEU:CD2	2:A:593:MPD:H51	1.70	1.18
1:A:401:GLU:HB2	1:A:402:PRO:HA	1.18	1.15
1:A:95:ILE:HG23	1:A:301:PRO:HD2	1.18	1.14
1:A:112:LEU:HG	5:A:775:HOH:O	1.46	1.14
1:A:148:LYS:HE2	5:A:676:HOH:O	0.94	1.11
1:A:421:LEU:HD13	2:A:593:MPD:CM	1.82	1.08
1:A:433:LEU:HD22	2:A:593:MPD:H51	1.28	1.07
1:A:433:LEU:HD22	2:A:593:MPD:H53	1.36	1.07
1:A:421:LEU:HD13	2:A:593:MPD:HM3	1.37	1.07
1:A:69:GLY:HA3	1:A:103:ILE:HA	1.31	1.05
1:A:191:GLN:NE2	1:A:199:ARG:NH2	2.05	1.03
1:A:433:LEU:HD23	2:A:593:MPD:C5	1.88	1.03
1:A:414:PHE:CE2	1:A:436:TYR:CE2	2.47	1.02
1:A:90:ARG:NH2	1:A:96:ARG:H	1.60	1.00
1:A:107:VAL:O	1:A:108:THR:HB	1.62	0.99
1:A:414:PHE:HE2	1:A:436:TYR:CE2	1.80	0.98
1:A:421:LEU:CD1	2:A:593:MPD:CM	2.45	0.95
1:A:95:ILE:HG23	1:A:301:PRO:CD	1.96	0.94
1:A:401:GLU:HB2	1:A:402:PRO:CA	1.99	0.93
1:A:144:ILE:HG21	1:A:290:ARG:CD	1.99	0.92
1:A:433:LEU:CD2	2:A:593:MPD:H52	1.99	0.92
1:A:90:ARG:HH21	1:A:96:ARG:H	1.01	0.92
1:A:191:GLN:HE22	1:A:199:ARG:HH22	1.09	0.92
1:A:216:ARG:H	1:A:505:GLN:HE22	1.14	0.91
1:A:414:PHE:HE2	1:A:436:TYR:HE2	1.16	0.90
1:A:297:THR:H	1:A:300:MET:HE2	1.35	0.89
1:A:95:ILE:HG22	1:A:301:PRO:HD2	1.55	0.89
1:A:90:ARG:NH2	1:A:95:ILE:HG13	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HG21	1:A:290:ARG:HD2	1.53	0.89
1:A:264:ARG:HB2	1:A:267:GLU:HB2	1.55	0.88
1:A:260:GLY:HA2	1:A:332:SER:OG	1.75	0.87
1:A:458:MET:HE1	1:A:525:ARG:HA	1.55	0.86
1:A:90:ARG:HH21	1:A:96:ARG:N	1.76	0.83
1:A:88:ILE:O	1:A:88:ILE:HG22	1.77	0.83
1:A:261:CYS:SG	1:A:262:GLY:N	2.50	0.83
1:A:296:ASN:HA	1:A:300:MET:HE1	1.61	0.81
1:A:86:ASP:HB2	1:A:95:ILE:HD12	1.61	0.81
1:A:297:THR:H	1:A:300:MET:CE	1.95	0.80
1:A:401:GLU:CB	1:A:402:PRO:HA	2.08	0.79
1:A:433:LEU:HD23	2:A:593:MPD:H51	1.52	0.78
1:A:90:ARG:NH2	1:A:95:ILE:CG1	2.47	0.77
1:A:406:ASN:O	1:A:410:VAL:HG23	1.86	0.76
1:A:335:ARG:NE	1:A:335:ARG:HA	2.01	0.76
1:A:221:PHE:HA	1:A:459:ARG:HH21	1.49	0.75
1:A:96:ARG:HE	1:A:96:ARG:HA	1.50	0.75
1:A:216:ARG:H	1:A:505:GLN:NE2	1.83	0.75
1:A:84:ILE:HG13	1:A:293:LEU:HG	1.69	0.75
1:A:421:LEU:CD1	2:A:593:MPD:HM1	2.17	0.74
1:A:191:GLN:HE21	1:A:199:ARG:NH2	1.85	0.74
1:A:95:ILE:CD1	1:A:304:ALA:HB1	2.17	0.74
1:A:244:GLN:HE22	1:A:391:ALA:HB2	1.53	0.74
1:A:95:ILE:CG2	1:A:301:PRO:CD	2.58	0.73
1:A:338:GLU:O	1:A:338:GLU:OE2	2.07	0.73
1:A:421:LEU:HD13	2:A:593:MPD:HM1	1.69	0.73
1:A:433:LEU:HD23	2:A:593:MPD:H52	1.62	0.72
1:A:94:VAL:O	1:A:95:ILE:HB	1.88	0.72
1:A:574:LYS:HE2	5:A:737:HOH:O	1.91	0.70
1:A:147:HIS:HE1	1:A:318:TYR:OH	1.74	0.69
1:A:332:SER:H	2:A:592:MPD:HM3	1.58	0.69
1:A:95:ILE:HD13	1:A:304:ALA:CB	2.23	0.68
1:A:95:ILE:HD13	1:A:304:ALA:HB1	1.75	0.68
1:A:72:LEU:HD11	1:A:88:ILE:HG12	1.76	0.68
1:A:107:VAL:O	1:A:108:THR:CB	2.42	0.66
1:A:390:GLY:HA3	5:A:838:HOH:O	1.94	0.66
1:A:102:PHE:HD1	1:A:103:ILE:HG22	1.59	0.66
1:A:115:ASP:N	1:A:115:ASP:OD1	2.29	0.65
1:A:144:ILE:CG2	1:A:290:ARG:HD2	2.26	0.65
1:A:239:GLY:HA3	5:A:826:HOH:O	1.97	0.65
1:A:141:GLU:OE1	1:A:147:HIS:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ARG:NH2	5:A:772:HOH:O	2.30	0.65
1:A:421:LEU:CD1	2:A:593:MPD:HM3	2.18	0.64
1:A:79:ARG:O	1:A:79:ARG:NE	2.30	0.64
1:A:254:GLN:NE2	1:A:325:ASP:H	1.96	0.64
1:A:88:ILE:O	1:A:88:ILE:CG2	2.46	0.63
1:A:391:ALA:O	2:A:592:MPD:HM2	1.99	0.63
1:A:80:LEU:HD12	1:A:85:TYR:OH	1.99	0.63
1:A:390:GLY:CA	5:A:838:HOH:O	2.47	0.63
1:A:293:LEU:N	1:A:293:LEU:HD23	2.14	0.62
1:A:90:ARG:CZ	1:A:95:ILE:HG13	2.28	0.62
1:A:95:ILE:CD1	1:A:304:ALA:CB	2.77	0.61
1:A:74:VAL:HG13	1:A:195:VAL:CG1	2.30	0.61
1:A:494:VAL:HG11	1:A:531:TYR:HB2	1.83	0.61
1:A:456:LYS:O	1:A:459:ARG:HG3	2.00	0.61
1:A:226:LYS:NZ	5:A:645:HOH:O	2.34	0.61
1:A:249:LYS:HZ2	2:A:589:MPD:C3	2.14	0.60
1:A:556:ILE:O	1:A:559:MET:HG3	2.01	0.60
1:A:414:PHE:CE2	1:A:436:TYR:HE2	2.01	0.60
1:A:245:HIS:O	1:A:249:LYS:HG2	2.01	0.60
1:A:80:LEU:O	1:A:83:SER:HB3	2.01	0.60
1:A:95:ILE:HD11	1:A:304:ALA:HB1	1.85	0.59
1:A:254:GLN:HE22	1:A:325:ASP:H	1.49	0.59
1:A:338:GLU:O	1:A:338:GLU:CD	2.41	0.58
1:A:75:GLU:HB2	1:A:112:LEU:HD13	1.85	0.58
1:A:216:ARG:N	1:A:505:GLN:HE22	1.95	0.58
1:A:336:TRP:CH2	1:A:364:LEU:HD13	2.37	0.58
1:A:79:ARG:CD	1:A:79:ARG:O	2.52	0.58
1:A:112:LEU:HB3	5:A:851:HOH:O	2.05	0.57
2:A:592:MPD:O4	2:A:592:MPD:O2	2.19	0.57
1:A:79:ARG:HA	5:A:806:HOH:O	2.04	0.56
1:A:249:LYS:NZ	2:A:589:MPD:H11	2.21	0.56
2:A:593:MPD:HM1	2:A:593:MPD:O4	2.06	0.56
1:A:86:ASP:CB	1:A:95:ILE:HD12	2.36	0.56
1:A:250:TRP:CH2	1:A:281:PRO:HB2	2.40	0.56
1:A:297:THR:HG22	1:A:299:ASN:H	1.70	0.56
1:A:414:PHE:CE2	1:A:436:TYR:CD2	2.94	0.56
1:A:79:ARG:O	1:A:79:ARG:HD2	2.05	0.56
1:A:421:LEU:HD11	2:A:593:MPD:CM	2.35	0.56
1:A:456:LYS:HA	1:A:459:ARG:HG2	1.88	0.56
1:A:448:HIS:HE1	1:A:456:LYS:H	1.54	0.55
1:A:290:ARG:CZ	5:A:772:HOH:O	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:THR:HA	2:A:592:MPD:H13	1.87	0.55
1:A:394:PRO:HB3	1:A:398:ASP:O	2.06	0.55
1:A:201:TYR:CZ	2:A:594:MPD:HM1	2.43	0.54
1:A:84:ILE:CG1	1:A:293:LEU:HG	2.38	0.54
1:A:317:GLU:HA	1:A:320:ARG:HG2	1.89	0.54
1:A:95:ILE:HG21	1:A:300:MET:HB3	1.91	0.53
1:A:332:SER:H	2:A:592:MPD:CM	2.21	0.53
1:A:297:THR:HG21	1:A:299:ASN:OD1	2.08	0.52
1:A:254:GLN:O	1:A:290:ARG:NE	2.42	0.52
1:A:244:GLN:HE22	1:A:391:ALA:CB	2.23	0.52
1:A:458:MET:HE3	1:A:525:ARG:HG2	1.92	0.52
1:A:297:THR:CG2	1:A:299:ASN:OD1	2.58	0.52
1:A:96:ARG:HA	1:A:96:ARG:NE	2.23	0.51
1:A:88:ILE:HD13	1:A:97:GLU:OE1	2.11	0.51
1:A:148:LYS:CE	5:A:676:HOH:O	1.80	0.51
1:A:121:ILE:HG13	5:A:708:HOH:O	2.10	0.51
1:A:260:GLY:CA	1:A:332:SER:OG	2.54	0.50
1:A:90:ARG:NH2	1:A:95:ILE:HG12	2.26	0.50
1:A:459:ARG:HD3	1:A:460:ASP:OD1	2.12	0.50
1:A:297:THR:N	1:A:300:MET:HE2	2.15	0.50
1:A:249:LYS:HZ2	2:A:589:MPD:H11	1.75	0.50
1:A:421:LEU:HD11	2:A:593:MPD:HM1	1.90	0.50
1:A:79:ARG:HB2	1:A:118:TRP:HZ2	1.76	0.50
1:A:108:THR:HG22	1:A:108:THR:O	2.10	0.49
1:A:75:GLU:CB	1:A:112:LEU:HD13	2.43	0.49
1:A:108:THR:CG2	1:A:108:THR:O	2.60	0.49
1:A:89:GLN:NE2	1:A:111:ALA:HB1	2.27	0.49
1:A:336:TRP:HH2	1:A:364:LEU:HD13	1.77	0.49
1:A:212:ILE:HD11	1:A:446:TRP:CH2	2.48	0.49
1:A:359:TYR:O	1:A:363:LYS:HG3	2.13	0.49
1:A:293:LEU:H	1:A:293:LEU:HD23	1.77	0.49
1:A:333:THR:HG21	1:A:393:SER:O	2.13	0.48
2:A:590:MPD:HM1	2:A:590:MPD:O4	2.12	0.48
1:A:85:TYR:HB3	1:A:89:GLN:HA	1.94	0.48
1:A:426:HIS:HD2	5:A:832:HOH:O	1.97	0.47
1:A:95:ILE:CG2	1:A:300:MET:HB3	2.43	0.47
1:A:487:ARG:HD2	5:A:658:HOH:O	2.15	0.47
1:A:72:LEU:HD11	1:A:88:ILE:HG21	1.95	0.47
1:A:536:GLU:O	1:A:539:ASN:HB3	2.15	0.47
1:A:499:ARG:O	1:A:504:GLN:HG3	2.14	0.47
1:A:119:HIS:NE2	1:A:165:GLU:OE2	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:O	1:A:79:ARG:CB	2.63	0.46
1:A:80:LEU:HD11	1:A:89:GLN:NE2	2.30	0.46
1:A:79:ARG:HD3	5:A:771:HOH:O	2.16	0.46
1:A:245:HIS:CE1	1:A:278:LEU:HD13	2.51	0.46
1:A:293:LEU:N	1:A:293:LEU:CD2	2.78	0.46
1:A:144:ILE:HG21	1:A:290:ARG:HD3	1.91	0.45
1:A:300:MET:HB2	1:A:300:MET:HE2	1.71	0.45
1:A:458:MET:CE	1:A:525:ARG:HG2	2.47	0.45
1:A:240:LYS:HD2	1:A:417:LEU:HD22	1.98	0.44
1:A:390:GLY:N	5:A:838:HOH:O	2.51	0.44
2:A:594:MPD:O4	2:A:594:MPD:HM1	2.18	0.44
1:A:199:ARG:HG3	1:A:317:GLU:OE1	2.16	0.44
1:A:401:GLU:HB3	1:A:405:GLN:HB2	1.99	0.44
1:A:160:VAL:HG11	1:A:178:LYS:HE3	1.98	0.44
1:A:287:LEU:CD1	1:A:290:ARG:HH12	2.30	0.44
1:A:129:LYS:HB3	1:A:129:LYS:NZ	2.33	0.44
1:A:287:LEU:HD12	1:A:290:ARG:HH12	1.83	0.44
1:A:72:LEU:HD11	1:A:88:ILE:CG2	2.48	0.43
2:A:590:MPD:HM2	5:A:687:HOH:O	2.18	0.43
1:A:495:ALA:O	1:A:499:ARG:HG3	2.19	0.43
1:A:246:GLN:OE1	2:A:589:MPD:C1	2.67	0.43
1:A:88:ILE:CD1	1:A:97:GLU:OE1	2.67	0.42
1:A:425:ARG:HD3	1:A:427:PHE:HE1	1.84	0.42
1:A:286:PRO:HB2	1:A:288:MET:HG2	2.01	0.42
1:A:467:GLN:HG2	5:A:673:HOH:O	2.20	0.42
1:A:108:THR:O	1:A:109:ALA:HB3	2.19	0.42
1:A:380:ASP:OD2	1:A:382:ARG:HD3	2.19	0.42
2:A:590:MPD:HM3	5:A:847:HOH:O	2.20	0.42
1:A:317:GLU:O	1:A:320:ARG:HG3	2.19	0.41
1:A:79:ARG:NH1	5:A:771:HOH:O	2.39	0.41
1:A:441:ASP:HA	1:A:444:LYS:HD3	2.01	0.41
1:A:63:GLU:HA	1:A:64:PRO:HD3	1.71	0.41
1:A:80:LEU:HA	1:A:80:LEU:HD12	1.91	0.41
1:A:459:ARG:HB2	1:A:459:ARG:HE	1.59	0.41
1:A:532:ASP:OD2	2:A:590:MPD:H11	2.21	0.41
1:A:366:GLU:HA	5:A:748:HOH:O	2.19	0.41
1:A:221:PHE:CA	1:A:459:ARG:HH21	2.27	0.41
1:A:249:LYS:HZ2	2:A:589:MPD:H32	1.86	0.40
1:A:303:ALA:O	1:A:306:GLU:HB3	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:811:HOH:O	5:A:817:HOH:O[7_555]	1.52	0.68
5:A:745:HOH:O	5:A:820:HOH:O[7_555]	1.97	0.23
5:A:731:HOH:O	5:A:736:HOH:O[3_454]	1.98	0.22

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	508/588 (86%)	469 (92%)	27 (5%)	12 (2%)	7 5

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	ILE
1	A	108	THR
1	A	110	PRO
1	A	92	LEU
1	A	94	VAL
1	A	103	ILE
1	A	69	GLY
1	A	87	GLY
1	A	401	GLU
1	A	64	PRO
1	A	109	ALA
1	A	402	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	433/492 (88%)	397 (92%)	36 (8%)	14	15

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	68	THR
1	A	79	ARG
1	A	90	ARG
1	A	94	VAL
1	A	96	ARG
1	A	98	LYS
1	A	99	THR
1	A	108	THR
1	A	115	ASP
1	A	129	LYS
1	A	162	ILE
1	A	164	GLU
1	A	181	SER
1	A	204	LYS
1	A	209	VAL
1	A	240	LYS
1	A	244	GLN
1	A	293	LEU
1	A	320	ARG
1	A	326	VAL
1	A	335	ARG
1	A	338	GLU
1	A	360	LEU
1	A	364	LEU
1	A	366	GLU
1	A	421	LEU
1	A	433	LEU
1	A	459	ARG
1	A	465	LEU
1	A	467	GLN
1	A	484	LEU
1	A	493	LEU
1	A	550	LEU
1	A	554	GLU
1	A	585	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	147	HIS
1	A	191	GLN
1	A	244	GLN
1	A	245	HIS
1	A	254	GLN
1	A	266	ASN
1	A	426	HIS
1	A	448	HIS
1	A	467	GLN
1	A	504	GLN
1	A	505	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](#)

7 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	MPD	A	589	-	6,7,7	1.95	1 (16%)	7,10,10	0.96	1 (14%)
2	MPD	A	590	-	6,7,7	0.19	0	7,10,10	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TRS	A	591	-	7,7,7	0.93	1 (14%)	9,9,9	0.83	0
2	MPD	A	592	-	6,7,7	4.49	1 (16%)	7,10,10	1.13	1 (14%)
2	MPD	A	593	-	6,7,7	0.62	0	7,10,10	0.39	0
2	MPD	A	594	-	6,7,7	2.86	1 (16%)	7,10,10	1.12	1 (14%)
4	ACY	A	595	-	1,3,3	1.39	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	A	589	-	-	0/5/5/5	0/0/0/0
2	MPD	A	590	-	-	0/5/5/5	0/0/0/0
3	TRS	A	591	-	-	0/9/9/9	0/0/0/0
2	MPD	A	592	-	-	0/5/5/5	0/0/0/0
2	MPD	A	593	-	-	0/5/5/5	0/0/0/0
2	MPD	A	594	-	-	0/5/5/5	0/0/0/0
4	ACY	A	595	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	592	MPD	C5-C4	-10.98	1.05	1.51
2	A	594	MPD	C5-C4	-6.95	1.22	1.51
2	A	589	MPD	C5-C4	-4.67	1.31	1.51
3	A	591	TRS	C-N	-2.22	1.47	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	594	MPD	O4-C4-C5	-2.77	95.64	109.55
2	A	592	MPD	O4-C4-C5	-2.72	95.91	109.55
2	A	589	MPD	O4-C4-C5	2.34	121.28	109.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	589	MPD	5	0
2	A	590	MPD	4	0
2	A	592	MPD	5	0
2	A	593	MPD	18	0
2	A	594	MPD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	512/588 (87%)	0.79	65 (12%) 5 9	26, 50, 101, 120	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	ILE	23.4
1	A	107	VAL	14.8
1	A	399	PHE	11.1
1	A	61	PRO	8.7
1	A	62	GLY	8.6
1	A	337	ALA	8.4
1	A	404	VAL	8.3
1	A	103	ILE	7.9
1	A	397	GLY	7.9
1	A	100	GLY	7.5
1	A	99	THR	7.5
1	A	64	PRO	7.5
1	A	94	VAL	6.5
1	A	408	LEU	6.4
1	A	273	GLU	6.3
1	A	108	THR	6.2
1	A	396	GLY	5.8
1	A	395	PRO	5.6
1	A	398	ASP	5.4
1	A	65	VAL	5.4
1	A	400	SER	5.2
1	A	70	ALA	5.2
1	A	92	LEU	5.0
1	A	149	ILE	4.6
1	A	361	ALA	4.3
1	A	359	TYR	4.1
1	A	407	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	275	PHE	4.0
1	A	66	VAL	3.8
1	A	405	GLN	3.8
1	A	104	ALA	3.7
1	A	302	VAL	3.7
1	A	336	TRP	3.4
1	A	71	SER	3.4
1	A	588	ALA	3.4
1	A	264	ARG	3.2
1	A	358	ALA	3.2
1	A	299	ASN	3.1
1	A	587	GLY	3.0
1	A	143	SER	3.0
1	A	84	ILE	2.9
1	A	96	ARG	2.8
1	A	106	GLY	2.7
1	A	261	CYS	2.6
1	A	357	PRO	2.6
1	A	109	ALA	2.6
1	A	362	SER	2.6
1	A	297	THR	2.5
1	A	102	PHE	2.5
1	A	88	ILE	2.5
1	A	266	ASN	2.5
1	A	136	ILE	2.4
1	A	304	ALA	2.4
1	A	403	VAL	2.4
1	A	290	ARG	2.4
1	A	340	LEU	2.4
1	A	436	TYR	2.3
1	A	298	SER	2.3
1	A	584	LYS	2.2
1	A	80	LEU	2.2
1	A	303	ALA	2.2
1	A	401	GLU	2.1
1	A	91	PRO	2.1
1	A	409	ARG	2.0
1	A	220	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
2	MPD	A	589	8/8	0.76	0.34	7.47	58,63,65,67	0
2	MPD	A	590	8/8	0.65	0.36	5.05	78,81,83,83	0
2	MPD	A	592	8/8	0.70	0.41	4.53	94,95,95,95	0
3	TRS	A	591	8/8	0.51	0.42	4.42	91,91,92,92	0
2	MPD	A	593	8/8	0.89	0.34	4.13	78,83,85,86	0
2	MPD	A	594	8/8	0.66	0.45	-	71,73,76,76	0
4	ACY	A	595	4/4	0.76	0.31	-	102,102,102,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.