



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:54 am BST

PDB ID : 3P20
Title : Crystal structure of vanadate bound subunit A of the A1AO ATP synthase
Authors : Manimekalai, M.S.S.; Kumar, A.; Jeyakanthan, J.; Gruber, G.
Deposited on : 2010-10-01
Resolution : 2.85 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (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

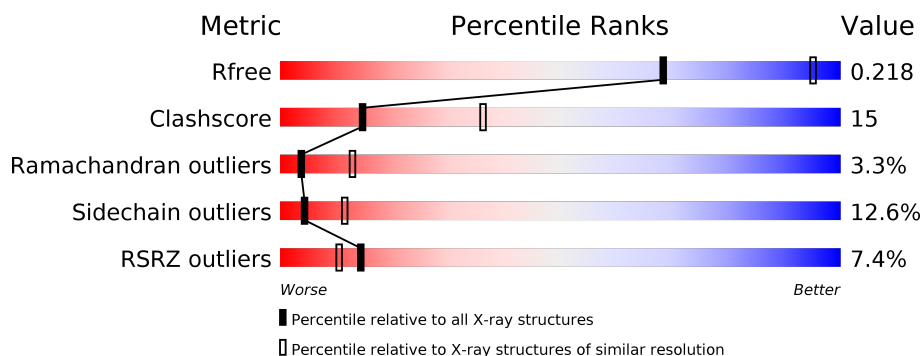
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 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	

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
3	ACY	A	593	-	-	X	-
3	ACY	A	600	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4237 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.

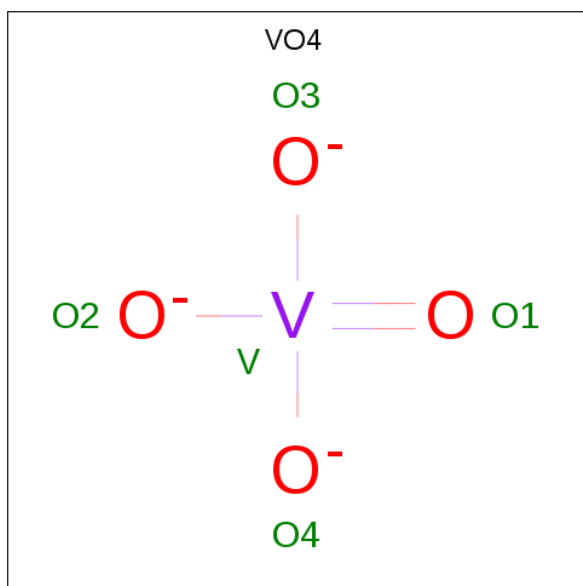
- Molecule 1 is a protein called V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	517	4086	2612	700	758	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is VANADATE ION (three-letter code: VO4) (formula: O₄V).



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

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



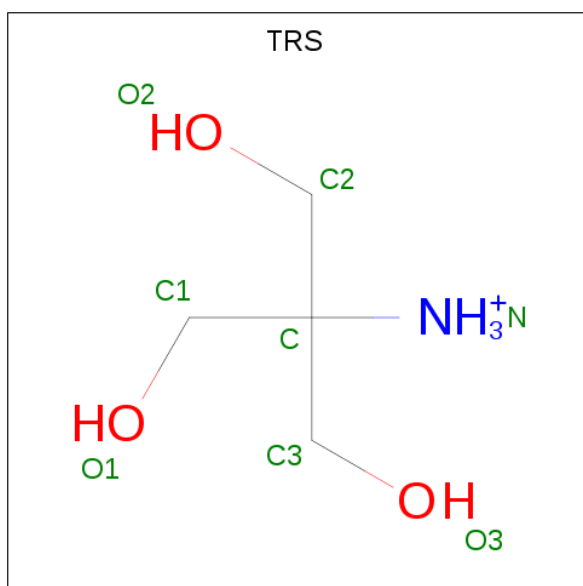
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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



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

- Molecule 5 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
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

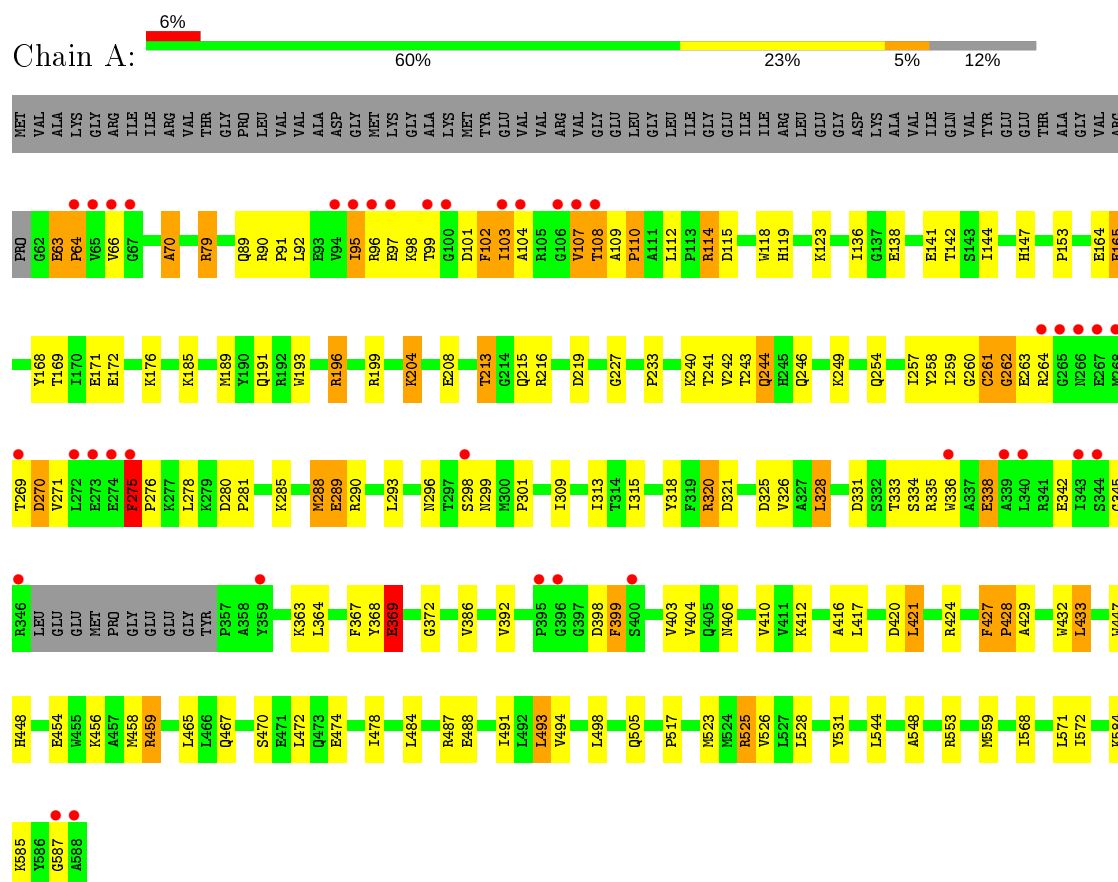
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total	O	0	0
			85	85		

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 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: 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, α , β , γ	127.55Å 127.55Å 104.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.25 – 2.85 29.25 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.25-2.85) 100.0 (29.25-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.210 , 0.246 0.206 , 0.218	Depositor DCC
R_{free} test set	1051 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4237	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, MPD, TRS, ACY

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	0.76	1/4174 (0.0%)	0.83	4/5653 (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	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	GLU	CG-CD	5.12	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	PHE	C-N-CD	-11.99	94.23	120.60
1	A	428	PRO	N-CA-C	-7.20	93.38	112.10
1	A	484	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	459	ARG	NE-CZ-NH1	-5.05	117.78	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	VAL	Peptide
1	A	233	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	427	PHE	Mainchain,Peptide
1	A	92	LEU	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	4086	0	4146	128	0
2	A	10	0	0	0	0
3	A	24	0	18	5	0
4	A	24	0	42	5	0
5	A	8	0	12	0	0
6	A	85	0	0	0	0
All	All	4237	0	4218	128	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 15.

All (128) 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:241:THR:HB	3:A:593:ACY:H2	1.32	1.11
1:A:142:THR:HB	1:A:289:GLU:HG3	1.26	1.10
1:A:216:ARG:H	1:A:505:GLN:HE22	1.08	0.94
1:A:254:GLN:NE2	1:A:325:ASP:H	1.66	0.92
1:A:261:CYS:HA	1:A:296:ASN:HB2	1.52	0.92
1:A:458:MET:HE1	1:A:525:ARG:HA	1.54	0.88
1:A:458:MET:HE1	1:A:525:ARG:HG2	1.57	0.86
1:A:196:ARG:HG3	1:A:196:ARG:HH11	1.39	0.86
1:A:144:ILE:HD12	1:A:289:GLU:HB3	1.56	0.86
1:A:142:THR:HB	1:A:289:GLU:CG	2.05	0.85
1:A:191:GLN:NE2	1:A:199:ARG:NH2	2.24	0.85
1:A:525:ARG:NH1	1:A:525:ARG:HG3	1.93	0.82
1:A:525:ARG:HG3	1:A:525:ARG:HH11	1.45	0.82
1:A:97:GLU:HG3	1:A:104:ALA:HB2	1.62	0.82
1:A:70:ALA:HB3	1:A:103:ILE:HG21	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:THR:HG22	1:A:215:GLN:H	1.45	0.81
1:A:216:ARG:H	1:A:505:GLN:NE2	1.78	0.81
1:A:70:ALA:CB	1:A:103:ILE:HG21	2.11	0.81
1:A:142:THR:CB	1:A:289:GLU:HG3	2.10	0.80
1:A:261:CYS:H	1:A:331:ASP:HB3	1.46	0.80
1:A:213:THR:HG23	1:A:215:GLN:HG2	1.62	0.80
1:A:254:GLN:HE22	1:A:325:ASP:H	1.28	0.79
1:A:448:HIS:HE1	1:A:456:LYS:H	1.32	0.77
1:A:244:GLN:HE21	1:A:244:GLN:H	1.33	0.76
1:A:216:ARG:N	1:A:505:GLN:HE22	1.85	0.74
1:A:191:GLN:NE2	1:A:199:ARG:HH22	1.85	0.74
1:A:196:ARG:HH11	1:A:196:ARG:CG	2.03	0.71
1:A:147:HIS:HE1	1:A:318:TYR:OH	1.74	0.70
1:A:70:ALA:HB3	1:A:103:ILE:CG2	2.22	0.69
1:A:398:ASP:O	1:A:399:PHE:HB2	1.93	0.69
1:A:97:GLU:HG3	1:A:104:ALA:CB	2.23	0.68
1:A:107:VAL:HG12	1:A:108:THR:H	1.58	0.67
1:A:458:MET:CE	1:A:525:ARG:HA	2.25	0.66
1:A:458:MET:HE1	1:A:525:ARG:CA	2.25	0.65
1:A:465:LEU:CD1	1:A:491:ILE:HG23	2.28	0.64
1:A:465:LEU:HD21	1:A:494:VAL:HG12	1.78	0.64
1:A:199:ARG:NH1	1:A:321:ASP:OD2	2.32	0.62
1:A:114:ARG:NH1	1:A:171:GLU:OE2	2.33	0.62
1:A:171:GLU:OE1	1:A:171:GLU:HA	1.99	0.61
1:A:406:ASN:ND2	4:A:595:MPD:O4	2.31	0.61
1:A:548:ALA:O	1:A:553:ARG:NH1	2.30	0.61
1:A:213:THR:HB	1:A:219:ASP:OD1	2.01	0.60
1:A:141:GLU:OE1	1:A:147:HIS:HD2	1.84	0.60
1:A:432:TRP:CD1	1:A:433:LEU:HD13	2.37	0.59
1:A:494:VAL:HG11	1:A:531:TYR:HB2	1.84	0.59
1:A:320:ARG:HG2	1:A:386:VAL:HG23	1.85	0.58
1:A:213:THR:CG2	1:A:215:GLN:H	2.15	0.58
1:A:364:LEU:O	1:A:367:PHE:HB3	2.03	0.58
1:A:241:THR:CB	3:A:593:ACY:H2	2.21	0.58
1:A:458:MET:HE1	1:A:525:ARG:CG	2.32	0.57
1:A:559:MET:CE	1:A:571:LEU:HD12	2.35	0.56
1:A:70:ALA:HB2	1:A:103:ILE:HG21	1.86	0.56
1:A:523:MET:HG2	1:A:559:MET:HG3	1.87	0.56
1:A:242:VAL:H	3:A:593:ACY:C	2.20	0.54
1:A:246:GLN:OE1	4:A:594:MPD:H13	2.07	0.54
1:A:191:GLN:HE22	1:A:199:ARG:HH22	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:NH1	1:A:196:ARG:CG	2.67	0.54
1:A:168:TYR:HD1	1:A:172:GLU:OE1	1.91	0.53
1:A:275:PHE:H	1:A:276:PRO:HD2	1.73	0.53
1:A:263:GLU:OE2	1:A:270:ASP:HB3	2.08	0.53
1:A:403:VAL:HG22	4:A:595:MPD:HM2	1.92	0.52
1:A:249:LYS:HE2	1:A:281:PRO:HG3	1.92	0.52
1:A:559:MET:HE3	1:A:571:LEU:HD12	1.91	0.52
1:A:261:CYS:SG	1:A:262:GLY:N	2.83	0.52
1:A:525:ARG:CG	1:A:525:ARG:NH1	2.66	0.51
1:A:526:VAL:HG11	1:A:559:MET:HE3	1.93	0.51
1:A:249:LYS:NZ	4:A:594:MPD:HM2	2.25	0.51
1:A:465:LEU:CD2	1:A:494:VAL:HG12	2.39	0.51
1:A:114:ARG:O	1:A:169:THR:HB	2.11	0.50
1:A:257:ILE:HB	1:A:328:LEU:HD12	1.92	0.50
1:A:191:GLN:HE22	1:A:199:ARG:NH2	2.07	0.50
1:A:153:PRO:HD2	1:A:191:GLN:HE22	1.77	0.50
1:A:259:ILE:HD13	1:A:309:ILE:HA	1.92	0.50
1:A:338:GLU:O	1:A:338:GLU:HG2	2.12	0.49
1:A:191:GLN:NE2	1:A:199:ARG:HH21	2.08	0.49
1:A:420:ASP:O	1:A:424:ARG:HG3	2.12	0.49
1:A:315:ILE:O	1:A:318:TYR:HB3	2.13	0.49
1:A:79:ARG:N	1:A:141:GLU:OE2	2.43	0.48
1:A:98:LYS:O	1:A:99:THR:HB	2.14	0.48
1:A:472:LEU:HD11	1:A:488:GLU:HG3	1.96	0.48
1:A:107:VAL:HG12	1:A:108:THR:N	2.28	0.47
1:A:164:GLU:O	1:A:165:GLU:C	2.51	0.47
1:A:63:GLU:HG2	1:A:64:PRO:CD	2.44	0.47
1:A:559:MET:HE2	1:A:559:MET:HB2	1.89	0.47
1:A:429:ALA:H	3:A:593:ACY:H3	1.78	0.47
1:A:244:GLN:NE2	1:A:244:GLN:H	2.08	0.47
1:A:97:GLU:H	1:A:301:PRO:HG2	1.80	0.47
1:A:261:CYS:HB3	1:A:331:ASP:HB3	1.98	0.46
1:A:147:HIS:CE1	1:A:318:TYR:OH	2.63	0.46
1:A:421:LEU:HD12	1:A:421:LEU:HA	1.68	0.46
1:A:123:LYS:HE3	1:A:138:GLU:HG3	1.96	0.46
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.81	0.46
1:A:249:LYS:HZ2	4:A:594:MPD:HM2	1.81	0.45
1:A:70:ALA:CB	1:A:103:ILE:CG2	2.86	0.45
1:A:493:LEU:HD12	1:A:544:LEU:HD11	1.99	0.45
1:A:472:LEU:HD21	1:A:488:GLU:CG	2.47	0.45
1:A:559:MET:HE2	1:A:568:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:O	1:A:335:ARG:HG3	2.15	0.44
1:A:526:VAL:HG22	1:A:572:ILE:HG13	1.99	0.44
1:A:63:GLU:HG2	1:A:64:PRO:HD3	2.00	0.44
1:A:114:ARG:HD2	1:A:171:GLU:HG2	1.99	0.44
1:A:79:ARG:HB2	1:A:118:TRP:HZ2	1.83	0.43
1:A:204:LYS:HD2	1:A:372:GLY:HA3	1.99	0.43
1:A:79:ARG:HB2	1:A:118:TRP:CZ2	2.53	0.43
1:A:448:HIS:CE1	1:A:456:LYS:H	2.23	0.43
1:A:119:HIS:NE2	1:A:165:GLU:OE2	2.46	0.43
1:A:392:VAL:CG1	1:A:404:VAL:HG12	2.49	0.43
1:A:176:LYS:HA	1:A:185:LYS:O	2.18	0.43
1:A:258:TYR:HE2	1:A:260:GLY:CA	2.32	0.43
1:A:398:ASP:O	1:A:399:PHE:CB	2.65	0.43
1:A:369:GLU:OE1	1:A:369:GLU:HA	2.19	0.42
1:A:368:TYR:HB2	1:A:410:VAL:HG11	2.01	0.42
1:A:153:PRO:HG2	1:A:193:TRP:CZ3	2.54	0.42
1:A:227:GLY:HA2	1:A:386:VAL:O	2.18	0.42
1:A:333:THR:O	1:A:335:ARG:HG2	2.19	0.42
1:A:447:TRP:CZ3	1:A:517:PRO:HB3	2.55	0.42
1:A:109:ALA:HA	1:A:110:PRO:HD3	1.92	0.41
1:A:258:TYR:HE2	1:A:260:GLY:HA2	1.86	0.41
1:A:102:PHE:HB2	1:A:103:ILE:H	1.69	0.41
1:A:280:ASP:HB3	1:A:285:LYS:O	2.21	0.41
1:A:275:PHE:HB3	1:A:288:MET:CE	2.50	0.41
1:A:465:LEU:HD12	1:A:491:ILE:HG23	2.01	0.41
1:A:429:ALA:H	3:A:593:ACY:CH3	2.33	0.41
1:A:338:GLU:O	1:A:338:GLU:CG	2.69	0.41
1:A:528:LEU:HA	1:A:528:LEU:HD23	1.71	0.40
1:A:90:ARG:HA	1:A:91:PRO:HD3	1.97	0.40
1:A:90:ARG:CZ	1:A:95:ILE:HG23	2.51	0.40
1:A:262:GLY:O	1:A:263:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	513/588 (87%)	454 (88%)	42 (8%)	17 (3%)	4	13

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	110	PRO
1	A	270	ASP
1	A	334	SER
1	A	478	ILE
1	A	585	LYS
1	A	587	GLY
1	A	428	PRO
1	A	64	PRO
1	A	70	ALA
1	A	208	GLU
1	A	399	PHE
1	A	416	ALA
1	A	584	LYS
1	A	275	PHE
1	A	345	GLY
1	A	262	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	438/493 (89%)	383 (87%)	55 (13%)	4	11

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	79	ARG

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Mol	Chain	Res	Type
1	A	89	GLN
1	A	95	ILE
1	A	96	ARG
1	A	101	ASP
1	A	102	PHE
1	A	103	ILE
1	A	108	THR
1	A	112	LEU
1	A	114	ARG
1	A	115	ASP
1	A	136	ILE
1	A	165	GLU
1	A	189	MET
1	A	196	ARG
1	A	204	LYS
1	A	213	THR
1	A	240	LYS
1	A	243	THR
1	A	244	GLN
1	A	261	CYS
1	A	264	ARG
1	A	269	THR
1	A	271	VAL
1	A	275	PHE
1	A	278	LEU
1	A	288	MET
1	A	289	GLU
1	A	290	ARG
1	A	293	LEU
1	A	298	SER
1	A	299	ASN
1	A	313	ILE
1	A	320	ARG
1	A	326	VAL
1	A	328	LEU
1	A	336	TRP
1	A	338	GLU
1	A	342	GLU
1	A	363	LYS
1	A	369	GLU
1	A	412	LYS
1	A	417	LEU

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Mol	Chain	Res	Type
1	A	421	LEU
1	A	433	LEU
1	A	454	GLU
1	A	459	ARG
1	A	467	GLN
1	A	470	SER
1	A	474	GLU
1	A	487	ARG
1	A	493	LEU
1	A	498	LEU
1	A	525	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) 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	299	ASN
1	A	406	ASN
1	A	448	HIS
1	A	505	GLN

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

12 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
4	MPD	A	594	-	7,7,7	0.31	0	9,10,10	0.75	0
4	MPD	A	595	-	7,7,7	0.59	0	9,10,10	0.77	0
2	VO4	A	589	-	1,4,4	4.94	1 (100%)	-		
4	MPD	A	592	-	7,7,7	0.50	0	9,10,10	0.61	0
3	ACY	A	591	-	1,3,3	1.45	0	0,3,3	0.00	-
5	TRS	A	598	-	7,7,7	0.50	0	9,9,9	0.72	0
3	ACY	A	599	-	1,3,3	1.80	0	0,3,3	0.00	-
3	ACY	A	596	-	1,3,3	0.91	0	0,3,3	0.00	-
3	ACY	A	600	-	1,3,3	1.63	0	0,3,3	0.00	-
3	ACY	A	593	-	1,3,3	1.38	0	0,3,3	0.00	-
2	VO4	A	590	-	1,4,4	4.80	1 (100%)	-		
3	ACY	A	597	-	1,3,3	1.88	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
4	MPD	A	594	-	-	1/5/5/5	-
4	MPD	A	595	-	-	0/5/5/5	-
5	TRS	A	598	-	-	3/9/9/9	-
4	MPD	A	592	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	589	VO4	O1-V	4.94	1.91	1.63
2	A	590	VO4	O1-V	4.80	1.91	1.63

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	598	TRS	C1-C-C3-O3
5	A	598	TRS	C2-C-C3-O3
5	A	598	TRS	N-C-C3-O3
4	A	592	MPD	CM-C2-C3-C4
4	A	594	MPD	O2-C2-C3-C4
4	A	592	MPD	O2-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	594	MPD	3	0
4	A	595	MPD	2	0
3	A	593	ACY	5	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	517/588 (87%)	0.00	38 (7%) 14 10	17, 41, 121, 158	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ARG	8.0
1	A	106	GLY	7.7
1	A	108	THR	7.1
1	A	66	VAL	6.5
1	A	95	ILE	5.7
1	A	268	MET	5.5
1	A	588	ALA	4.9
1	A	266	ASN	4.4
1	A	107	VAL	4.2
1	A	267	GLU	4.2
1	A	64	PRO	4.1
1	A	104	ALA	4.1
1	A	97	GLU	4.0
1	A	587	GLY	4.0
1	A	269	THR	3.9
1	A	65	VAL	3.8
1	A	100	GLY	3.6
1	A	94	VAL	3.3
1	A	67	GLY	3.1
1	A	275	PHE	2.9
1	A	274	GLU	2.9
1	A	273	GLU	2.8
1	A	344	SER	2.8
1	A	103	ILE	2.8
1	A	336	TRP	2.7
1	A	396	GLY	2.7
1	A	400	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	272	LEU	2.5
1	A	265	GLY	2.5
1	A	359	TYR	2.5
1	A	340	LEU	2.4
1	A	343	ILE	2.4
1	A	339	ALA	2.3
1	A	99	THR	2.3
1	A	264	ARG	2.2
1	A	298	SER	2.2
1	A	395	PRO	2.1
1	A	346	ARG	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, 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	B-factors(Å ²)	Q<0.9
3	ACY	A	597	4/4	0.75	0.33	75,75,75,75	0
3	ACY	A	600	4/4	0.77	0.42	71,71,71,71	0
2	VO4	A	589	5/5	0.82	0.32	80,81,81,81	0
3	ACY	A	599	4/4	0.86	0.19	88,89,89,89	0
3	ACY	A	593	4/4	0.88	0.28	57,58,58,59	0
4	MPD	A	592	8/8	0.89	0.27	60,61,62,62	0
2	VO4	A	590	5/5	0.89	0.24	83,84,85,86	0
3	ACY	A	591	4/4	0.89	0.73	81,81,82,82	0
4	MPD	A	595	8/8	0.91	0.33	60,61,63,64	0
4	MPD	A	594	8/8	0.92	0.27	63,63,65,66	0
5	TRS	A	598	8/8	0.94	0.26	64,65,65,65	0
3	ACY	A	596	4/4	0.94	0.15	56,56,56,57	0

6.5 Other polymers

There are no such residues in this entry.