



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:57 am BST

PDB ID : 3SDZ
Title : Structural characterization of the subunit A mutant F427W of the A-ATP synthase from *Pyrococcus horikoshii*
Authors : Tadwal, V.S.; Manimekalai, M.S.S.; Balakrishna, A.M.; Gruber, G.
Deposited on : 2011-06-09
Resolution : 2.53 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

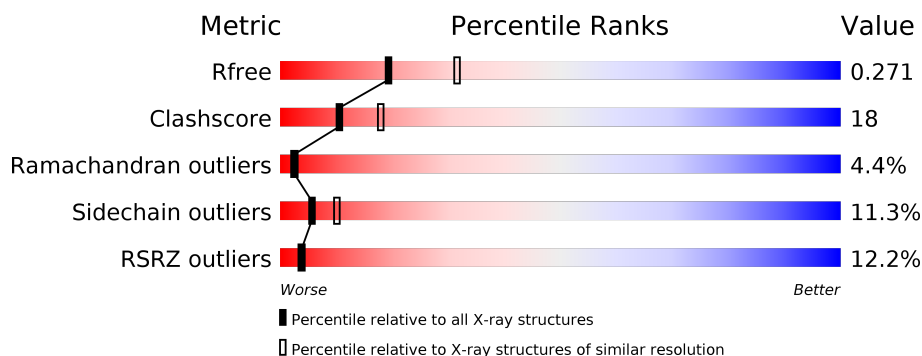
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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
4	TRS	A	599	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4701 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.

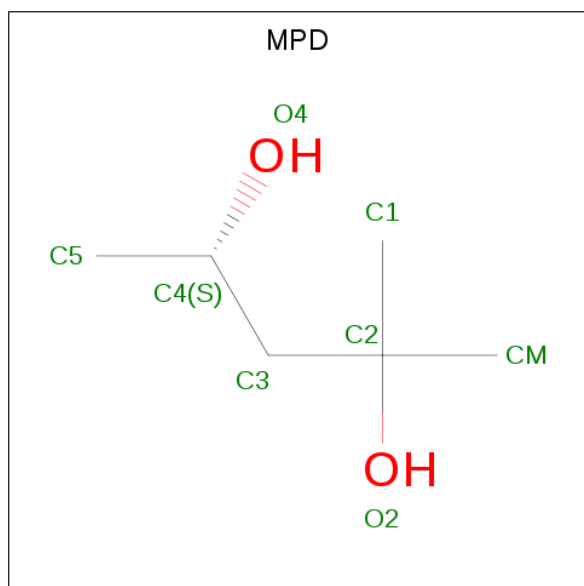
- Molecule 1 is a protein called V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	2	0
			4332	2772	734	809	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	427	TRP	PHE	ENGINEERED MUTATION	UNP O57728

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



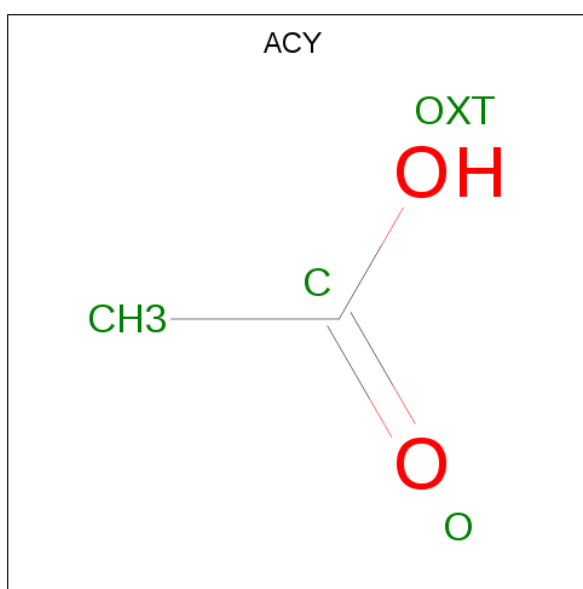
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		

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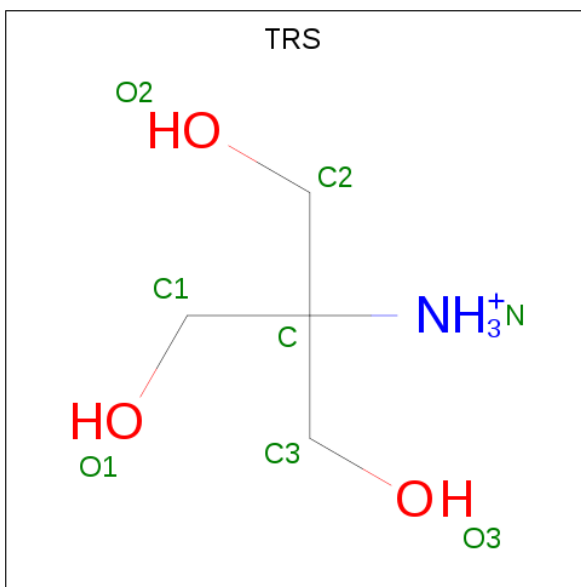
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		

- 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		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	273	Total	O	0	0
			273	273		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.88Å 127.88Å 105.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.17 – 2.53 26.17 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.17-2.53) 99.8 (26.17-2.53)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.200 , 0.266 0.205 , 0.271	Depositor DCC
R_{free} test set	1513 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.9	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	0.94	EDS
Total number of atoms	4701	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: 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	0.94	1/4431 (0.0%)	0.97	9/6005 (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	454	GLU	CG-CD	-6.43	1.42	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	ARG	NE-CZ-NH2	-13.90	113.35	120.30
1	A	199	ARG	NE-CZ-NH2	-13.55	113.53	120.30
1	A	499	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	199	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	373	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	373	ARG	CG-CD-NE	-6.29	98.58	111.80
1	A	553	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	493	LEU	CA-CB-CG	5.73	128.49	115.30
1	A	458	MET	CG-SD-CE	-5.19	91.89	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	PRO	Peptide
1	A	263	GLU	Peptide
1	A	264	ARG	Peptide
1	A	401	GLU	Peptide
1	A	406	ASN	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	4332	0	4378	153	1
2	A	48	0	78	16	0
3	A	24	0	18	1	0
4	A	24	0	36	2	0
5	A	273	0	0	14	0
All	All	4701	0	4510	165	1

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 18.

All (165) 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	1.35	1.21
1:A:235:PRO:HB3	1:A:240:LYS:HE3	1.06	1.03
1:A:191:GLN:NE2	1:A:199:ARG:NH2	2.10	0.99
1:A:264:ARG:HG2	1:A:265:GLY:H	1.24	0.98
1:A:249:LYS:HE2	2:A:589:MPD:H32	1.44	0.97
1:A:114:ARG:NE	1:A:170:ILE:HD11	1.82	0.95
1:A:464:ALA:HB3	2:A:592:MPD:H52	1.52	0.92
1:A:235:PRO:CB	1:A:240:LYS:HE3	1.98	0.91
1:A:363:LYS:O	1:A:366:GLU:HB3	1.70	0.91
1:A:75:GLU:H	1:A:89:GLN:HE22	1.18	0.91
1:A:573:ASP:O	1:A:577[A]:GLU:HG2	1.73	0.87
1:A:36:LEU:HD22	1:A:51:GLN:HG3	1.57	0.86
1:A:526:VAL:HG11	1:A:559:MET:HE3	1.59	0.82
1:A:406:ASN:HB3	1:A:409:ARG:HB2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:H	1:A:505:GLN:HE22	1.23	0.82
1:A:120:PHE:HB2	1:A:189:MET:CE	2.13	0.79
1:A:191:GLN:HE22	1:A:199:ARG:HH22	1.31	0.79
1:A:32:GLY:HA3	1:A:301:PRO:HG3	1.66	0.77
1:A:559:MET:CE	1:A:571:LEU:HD12	2.13	0.77
1:A:264:ARG:CG	1:A:265:GLY:H	1.98	0.77
1:A:256:VAL:HG23	1:A:290:ARG:HH21	1.50	0.75
1:A:74:VAL:CG1	1:A:76:LEU:HD21	2.16	0.74
1:A:97:GLU:HG2	1:A:101:ASP:HA	1.68	0.74
1:A:147:HIS:HE1	1:A:318:TYR:OH	1.71	0.73
1:A:526:VAL:HG11	1:A:559:MET:CE	2.18	0.73
1:A:424:ARG:HD3	5:A:738:HOH:O	1.87	0.73
1:A:245:HIS:O	1:A:249:LYS:HG2	1.86	0.73
1:A:120:PHE:HB2	1:A:189:MET:HE3	1.72	0.71
1:A:559:MET:HE1	1:A:571:LEU:HD12	1.71	0.71
1:A:147:HIS:CE1	1:A:318:TYR:OH	2.44	0.70
2:A:592:MPD:H11	2:A:592:MPD:O4	1.92	0.70
1:A:191:GLN:HE21	1:A:199:ARG:NH2	1.90	0.70
1:A:264:ARG:HG2	1:A:265:GLY:N	2.04	0.70
2:A:589:MPD:O4	2:A:589:MPD:H11	1.92	0.69
1:A:494:VAL:HG11	1:A:531:TYR:HB2	1.73	0.69
2:A:590:MPD:H11	2:A:590:MPD:O4	1.92	0.69
1:A:273:GLU:HA	1:A:276:PRO:HD2	1.74	0.68
1:A:448:HIS:HE1	1:A:456:LYS:H	1.42	0.67
1:A:216:ARG:H	1:A:505:GLN:NE2	1.93	0.65
1:A:241:THR:O	1:A:245:HIS:HB2	1.95	0.65
2:A:591:MPD:O4	2:A:591:MPD:H11	1.95	0.65
1:A:234:GLY:HA3	1:A:393:SER:HB3	1.78	0.65
1:A:257:ILE:HB	1:A:328:LEU:HD12	1.79	0.65
2:A:602:MPD:HM1	2:A:602:MPD:O4	1.96	0.64
1:A:584:LYS:C	1:A:586:TYR:H	1.99	0.64
1:A:245:HIS:NE2	2:A:589:MPD:H52	2.13	0.64
1:A:143:SER:OG	1:A:289:GLU:OE2	2.16	0.64
1:A:262:GLY:HA3	1:A:296:ASN:O	1.99	0.63
1:A:74:VAL:HG11	1:A:76:LEU:HD21	1.79	0.63
1:A:234:GLY:HA3	1:A:393:SER:CB	2.29	0.62
1:A:394:PRO:HB3	1:A:398:ASP:O	1.99	0.62
1:A:75:GLU:OE1	1:A:114:ARG:NH2	2.33	0.62
1:A:401:GLU:HA	1:A:405:GLN:HB2	1.82	0.62
1:A:373:ARG:HD2	5:A:631:HOH:O	2.00	0.61
1:A:546:GLU:HG3	1:A:582:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ALA:HB2	1:A:538:ILE:CD1	2.30	0.60
1:A:585:LYS:O	1:A:585:LYS:CG	2.50	0.60
1:A:536:GLU:O	1:A:540:ARG:HG3	2.01	0.59
1:A:531:TYR:OH	2:A:592:MPD:H11	2.03	0.59
1:A:28:VAL:O	1:A:34:LEU:HD21	2.02	0.58
1:A:275:PHE:HE1	3:A:598:ACY:OXT	1.86	0.58
1:A:420:ASP:OD1	1:A:423:ARG:NH2	2.33	0.58
1:A:114:ARG:CD	1:A:170:ILE:HD11	2.34	0.58
1:A:477:ARG:HD3	5:A:705:HOH:O	2.04	0.57
1:A:401:GLU:HB3	1:A:402:PRO:CD	2.35	0.57
1:A:233:PRO:O	1:A:234:GLY:O	2.22	0.57
1:A:74:VAL:CG1	1:A:76:LEU:CD2	2.82	0.57
1:A:204:LYS:HD2	1:A:372:GLY:HA3	1.86	0.56
2:A:591:MPD:HM2	5:A:759:HOH:O	2.04	0.56
2:A:594:MPD:O4	2:A:594:MPD:H11	2.06	0.56
1:A:254:GLN:HE22	1:A:325:ASP:H	1.54	0.55
1:A:61:PRO:HD2	1:A:65:VAL:HG23	1.87	0.55
1:A:302:VAL:HG13	5:A:825:HOH:O	2.07	0.55
1:A:93:GLU:HG3	1:A:107:VAL:HB	1.89	0.55
1:A:363:LYS:O	1:A:366:GLU:CB	2.48	0.55
1:A:399:PHE:HA	1:A:404:VAL:HG21	1.87	0.55
2:A:590:MPD:C1	2:A:590:MPD:O4	2.43	0.55
1:A:153:PRO:HD3	1:A:191:GLN:HE22	1.71	0.55
1:A:373:ARG:HG3	1:A:385:SER:HB3	1.89	0.54
1:A:559:MET:CE	1:A:571:LEU:CD1	2.83	0.54
1:A:46:ASP:O	1:A:47:LYS:HB3	2.08	0.54
2:A:589:MPD:O4	2:A:589:MPD:C1	2.43	0.54
1:A:585:LYS:O	1:A:585:LYS:HG2	2.08	0.53
1:A:264:ARG:CG	1:A:265:GLY:N	2.68	0.53
2:A:592:MPD:O4	2:A:592:MPD:C1	2.43	0.53
1:A:102:PHE:HD1	1:A:269:THR:HB	1.73	0.53
1:A:490:ALA:HB2	1:A:538:ILE:HD12	1.92	0.52
1:A:109:ALA:HB1	1:A:110:PRO:HD2	1.90	0.52
1:A:245:HIS:CD2	1:A:249:LYS:HD3	2.45	0.51
1:A:464:ALA:CB	2:A:592:MPD:H52	2.33	0.51
2:A:591:MPD:C1	2:A:591:MPD:O4	2.58	0.51
1:A:426:HIS:HE1	5:A:612:HOH:O	1.92	0.51
1:A:360:LEU:C	1:A:362:SER:H	2.13	0.51
1:A:559:MET:HE2	1:A:571:LEU:CD1	2.42	0.50
1:A:240:LYS:O	1:A:244:GLN:HB2	2.12	0.50
1:A:33:GLU:HG2	1:A:34:LEU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:TRP:O	1:A:504:GLN:HA	2.12	0.50
1:A:273:GLU:HA	1:A:276:PRO:CD	2.39	0.49
1:A:114:ARG:HE	1:A:170:ILE:HD11	1.74	0.48
1:A:44:GLU:HG3	1:A:54:GLU:H	1.79	0.48
1:A:262:GLY:CA	1:A:296:ASN:O	2.61	0.48
1:A:254:GLN:NE2	1:A:325:ASP:H	2.11	0.48
1:A:427:TRP:HA	1:A:428:PRO:C	2.34	0.48
1:A:584:LYS:O	1:A:586:TYR:N	2.47	0.47
1:A:87:GLY:HA3	1:A:304:ALA:O	2.13	0.47
1:A:584:LYS:C	1:A:586:TYR:N	2.66	0.47
1:A:63:GLU:O	1:A:65:VAL:N	2.47	0.47
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.66	0.47
1:A:380:ASP:OD2	1:A:382:ARG:HD3	2.14	0.47
1:A:236:PHE:CB	5:A:860:HOH:O	2.63	0.46
1:A:216:ARG:N	1:A:505:GLN:HE22	2.02	0.46
1:A:249:LYS:HZ2	1:A:281:PRO:HG3	1.81	0.46
1:A:102:PHE:HB2	1:A:269:THR:HG22	1.97	0.46
1:A:362:SER:HB2	5:A:839:HOH:O	2.15	0.46
1:A:236:PHE:HB2	5:A:860:HOH:O	2.15	0.46
1:A:535:MET:O	1:A:539:ASN:HB2	2.16	0.45
1:A:581:GLU:HA	1:A:584:LYS:HZ2	1.80	0.45
1:A:394:PRO:C	1:A:396:GLY:H	2.20	0.45
1:A:402:PRO:O	1:A:405:GLN:HB3	2.17	0.45
1:A:95:ILE:HB	1:A:103:ILE:O	2.17	0.45
1:A:237:GLY:O	1:A:239:GLY:N	2.45	0.45
1:A:232:ILE:HG13	1:A:417:LEU:HD22	1.99	0.45
1:A:232:ILE:O	1:A:391:ALA:HA	2.17	0.45
1:A:232:ILE:CG1	1:A:417:LEU:HD22	2.46	0.45
1:A:428:PRO:HD2	5:A:709:HOH:O	2.16	0.45
1:A:76:LEU:O	1:A:190:TYR:HA	2.17	0.44
1:A:275:PHE:N	1:A:276:PRO:CD	2.81	0.44
1:A:53:TYR:CE2	1:A:56:THR:HA	2.53	0.44
1:A:529:ASN:O	1:A:533:LYS:HG2	2.17	0.44
1:A:107:VAL:HG23	5:A:757:HOH:O	2.17	0.44
1:A:420:ASP:O	1:A:424:ARG:HG3	2.18	0.44
1:A:585:LYS:CE	1:A:588:ALA:HB3	2.47	0.44
1:A:421:LEU:HD12	1:A:421:LEU:HA	1.87	0.43
1:A:564:ASP:OD1	1:A:566:SER:OG	2.33	0.43
1:A:559:MET:HE2	1:A:571:LEU:HD12	1.93	0.43
1:A:72:LEU:HD12	5:A:819:HOH:O	2.18	0.43
1:A:236:PHE:CE2	1:A:238:SER:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:HIS:O	1:A:249:LYS:CG	2.62	0.43
1:A:201:TYR:CE1	4:A:599:TRS:H32	2.53	0.43
1:A:249:LYS:NZ	1:A:281:PRO:HG3	2.34	0.43
1:A:465:LEU:HD21	1:A:531:TYR:CE1	2.53	0.43
1:A:256:VAL:HG23	1:A:290:ARG:NH2	2.26	0.42
1:A:114:ARG:NE	1:A:170:ILE:CD1	2.69	0.42
1:A:237:GLY:HA2	5:A:608:HOH:O	2.18	0.42
1:A:126:VAL:HA	1:A:159:ILE:HG22	2.02	0.42
1:A:36:LEU:O	1:A:42:ARG:O	2.37	0.42
1:A:374:VAL:O	1:A:383:VAL:HA	2.20	0.42
1:A:559:MET:HE2	1:A:559:MET:HB3	1.70	0.42
1:A:171:GLU:O	1:A:188:LYS:HE2	2.20	0.42
1:A:577[A]:GLU:H	1:A:577[A]:GLU:HG2	1.56	0.41
1:A:285:LYS:HG2	1:A:285:LYS:H	1.71	0.41
1:A:499:ARG:O	1:A:504:GLN:HG3	2.20	0.41
1:A:206:PRO:O	1:A:207:PRO:C	2.55	0.41
1:A:90:ARG:HA	1:A:91:PRO:HD3	1.87	0.41
4:A:601:TRS:O1	4:A:601:TRS:O2	2.31	0.41
1:A:499:ARG:NH2	5:A:811:HOH:O	2.54	0.41
1:A:36:LEU:HD11	1:A:46:ASP:HB2	2.02	0.41
1:A:273:GLU:HA	1:A:276:PRO:HG2	2.02	0.41
1:A:231:ALA:HA	1:A:390:GLY:O	2.21	0.41
1:A:331:ASP:HA	1:A:391:ALA:HB3	2.03	0.41
1:A:245:HIS:HD2	1:A:249:LYS:HD3	1.83	0.41
1:A:394:PRO:C	1:A:396:GLY:N	2.75	0.40
1:A:270:ASP:O	1:A:274:GLU:HB2	2.20	0.40
1:A:114:ARG:HD3	1:A:170:ILE:HD11	2.02	0.40
1:A:262:GLY:O	1:A:264:ARG:HA	2.22	0.40

All (1) 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)
1:A:488:GLU:OE1	1:A:506:ASP:OD2[3_444]	2.18	0.02

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	546/588 (93%)	478 (88%)	44 (8%)	24 (4%)	2 2

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	VAL
1	A	64	PRO
1	A	234	GLY
1	A	235	PRO
1	A	264	ARG
1	A	358	ALA
1	A	394	PRO
1	A	401	GLU
1	A	402	PRO
1	A	27	GLU
1	A	37	ILE
1	A	97	GLU
1	A	262	GLY
1	A	585	LYS
1	A	100	GLY
1	A	236	PHE
1	A	273	GLU
1	A	335	ARG
1	A	94	VAL
1	A	95	ILE
1	A	47	LYS
1	A	331	ASP
1	A	396	GLY
1	A	587	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	462/492 (94%)	409 (88%)	53 (12%)	5 10

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	TYR
1	A	30	ARG
1	A	37	ILE
1	A	41	ILE
1	A	47	LYS
1	A	51	GLN
1	A	54	GLU
1	A	60	ARG
1	A	71	SER
1	A	74	VAL
1	A	93	GLU
1	A	97	GLU
1	A	105	ARG
1	A	108	THR
1	A	112	LEU
1	A	114	ARG
1	A	159	ILE
1	A	178	LYS
1	A	181	SER
1	A	196	ARG
1	A	204	LYS
1	A	232	ILE
1	A	236	PHE
1	A	243	THR
1	A	249	LYS
1	A	264	ARG
1	A	269	THR
1	A	270	ASP
1	A	272	LEU
1	A	273	GLU

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Mol	Chain	Res	Type
1	A	274	GLU
1	A	280	ASP
1	A	285	LYS
1	A	290	ARG
1	A	320	ARG
1	A	326	VAL
1	A	331	ASP
1	A	359	TYR
1	A	393	SER
1	A	417	LEU
1	A	421	LEU
1	A	433	LEU
1	A	445	ASP
1	A	454	GLU
1	A	465	LEU
1	A	467	GLN
1	A	477	ARG
1	A	484	LEU
1	A	493	LEU
1	A	538	ILE
1	A	539	ASN
1	A	577[A]	GLU
1	A	577[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	147	HIS
1	A	191	GLN
1	A	254	GLN
1	A	426	HIS
1	A	448	HIS
1	A	504	GLN
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 [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](#)

15 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	590	-	7,7,7	2.94	1 (14%)	9,10,10	3.44	3 (33%)
3	ACY	A	595	-	1,3,3	1.71	0	0,3,3	0.00	-
2	MPD	A	594	-	7,7,7	0.27	0	9,10,10	0.22	0
4	TRS	A	599	-	7,7,7	0.30	0	9,9,9	0.71	0
3	ACY	A	597	-	1,3,3	1.66	0	0,3,3	0.00	-
2	MPD	A	589	-	7,7,7	2.94	1 (14%)	9,10,10	3.45	3 (33%)
4	TRS	A	601	-	7,7,7	0.42	0	9,9,9	1.22	1 (11%)
2	MPD	A	592	-	7,7,7	2.94	1 (14%)	9,10,10	3.44	3 (33%)
3	ACY	A	603	-	1,3,3	1.61	0	0,3,3	0.00	-
3	ACY	A	598	-	1,3,3	1.51	0	0,3,3	0.00	-
2	MPD	A	602	-	7,7,7	1.22	2 (28%)	9,10,10	0.22	0
3	ACY	A	593	-	1,3,3	1.76	0	0,3,3	0.00	-
2	MPD	A	591	-	7,7,7	0.28	0	9,10,10	0.22	0
4	TRS	A	600	-	7,7,7	0.44	0	9,9,9	0.81	0
3	ACY	A	596	-	1,3,3	1.80	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	590	-	-	0/5/5/5	-
4	TRS	A	601	-	-	6/9/9/9	-
2	MPD	A	594	-	-	0/5/5/5	-
4	TRS	A	599	-	-	6/9/9/9	-
2	MPD	A	589	-	-	0/5/5/5	-
4	TRS	A	600	-	-	7/9/9/9	-
2	MPD	A	592	-	-	0/5/5/5	-
2	MPD	A	602	-	-	0/5/5/5	-
2	MPD	A	591	-	-	0/5/5/5	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	590	MPD	O4-C4	-7.66	1.10	1.43
2	A	589	MPD	O4-C4	-7.65	1.10	1.43
2	A	592	MPD	O4-C4	-7.65	1.10	1.43
2	A	602	MPD	C5-C4	-2.28	1.41	1.51
2	A	602	MPD	O4-C4	2.24	1.52	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	589	MPD	O4-C4-C3	-9.09	74.65	111.36
2	A	592	MPD	O4-C4-C3	-9.09	74.67	111.36
2	A	590	MPD	O4-C4-C3	-9.08	74.70	111.36
2	A	589	MPD	C5-C4-C3	3.57	128.52	111.69
2	A	590	MPD	C5-C4-C3	3.56	128.49	111.69
2	A	592	MPD	C5-C4-C3	3.56	128.48	111.69
2	A	589	MPD	O2-C2-CM	-2.18	101.09	108.08
2	A	592	MPD	O2-C2-CM	-2.18	101.09	108.08
2	A	590	MPD	O2-C2-CM	-2.18	101.09	108.08
4	A	601	TRS	O3-C3-C	2.05	117.48	111.00

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	599	TRS	N-C-C2-O2
4	A	599	TRS	C2-C-C3-O3
4	A	599	TRS	N-C-C3-O3
4	A	601	TRS	C1-C-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	601	TRS	N-C-C2-O2
4	A	600	TRS	C2-C-C1-O1
4	A	599	TRS	C1-C-C3-O3
4	A	601	TRS	C2-C-C1-O1
4	A	601	TRS	N-C-C1-O1
4	A	601	TRS	C3-C-C2-O2
4	A	600	TRS	N-C-C1-O1
4	A	600	TRS	N-C-C3-O3
4	A	599	TRS	C1-C-C2-O2
4	A	601	TRS	C3-C-C1-O1
4	A	600	TRS	C3-C-C1-O1
4	A	600	TRS	C1-C-C3-O3
4	A	599	TRS	C3-C-C2-O2
4	A	600	TRS	N-C-C2-O2
4	A	600	TRS	C2-C-C3-O3

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	590	MPD	2	0
2	A	594	MPD	1	0
4	A	599	TRS	1	0
2	A	589	MPD	4	0
4	A	601	TRS	1	0
2	A	592	MPD	5	0
3	A	598	ACY	1	0
2	A	602	MPD	1	0
2	A	591	MPD	3	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	548/588 (93%)	0.40	67 (12%) 4 4	24, 51, 126, 165	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	THR	9.6
1	A	100	GLY	8.9
1	A	356	TYR	8.3
1	A	25	MET	8.1
1	A	102	PHE	7.7
1	A	37	ILE	7.2
1	A	336	TRP	6.4
1	A	588	ALA	6.3
1	A	394	PRO	6.2
1	A	59	VAL	6.1
1	A	66	VAL	6.0
1	A	359	TYR	5.8
1	A	29	VAL	5.1
1	A	264	ARG	5.0
1	A	41	ILE	4.7
1	A	95	ILE	4.6
1	A	273	GLU	4.5
1	A	399	PHE	4.4
1	A	101	ASP	4.4
1	A	395	PRO	4.3
1	A	396	GLY	4.3
1	A	50	ILE	4.2
1	A	96	ARG	4.1
1	A	94	VAL	4.0
1	A	98	LYS	3.9
1	A	333	THR	3.9
1	A	56	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	235	PRO	3.8
1	A	400	SER	3.7
1	A	404	VAL	3.7
1	A	402	PRO	3.6
1	A	393	SER	3.5
1	A	65	VAL	3.4
1	A	46	ASP	3.3
1	A	51	GLN	3.2
1	A	108	THR	3.2
1	A	362	SER	3.1
1	A	26	TYR	3.1
1	A	337	ALA	3.1
1	A	38	GLY	3.0
1	A	47	LYS	3.0
1	A	32	GLY	3.0
1	A	60	ARG	3.0
1	A	58	GLY	2.9
1	A	584	LYS	2.8
1	A	45	GLY	2.8
1	A	110	PRO	2.8
1	A	398	ASP	2.7
1	A	266	ASN	2.7
1	A	299	ASN	2.6
1	A	49	VAL	2.6
1	A	76	LEU	2.6
1	A	97	GLU	2.6
1	A	61	PRO	2.5
1	A	78	PRO	2.5
1	A	335	ARG	2.5
1	A	67	GLY	2.3
1	A	35	GLY	2.3
1	A	397	GLY	2.3
1	A	361	ALA	2.2
1	A	36	LEU	2.2
1	A	357	PRO	2.2
1	A	298	SER	2.2
1	A	389	ILE	2.1
1	A	405	GLN	2.1
1	A	53	TYR	2.1
1	A	44	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
4	TRS	A	599	8/8	0.64	0.48	86,88,89,89	0
2	MPD	A	594	8/8	0.69	0.31	88,90,91,92	0
4	TRS	A	601	8/8	0.74	0.29	74,76,77,77	0
3	ACY	A	593	4/4	0.79	0.22	74,74,75,75	0
3	ACY	A	597	4/4	0.79	0.25	121,121,121,121	0
2	MPD	A	589	8/8	0.82	0.28	50,54,60,62	0
2	MPD	A	602	8/8	0.83	0.23	90,91,91,92	0
2	MPD	A	592	8/8	0.85	0.27	50,54,60,62	0
3	ACY	A	598	4/4	0.86	0.41	98,98,98,98	0
2	MPD	A	590	8/8	0.87	0.22	50,54,60,62	0
2	MPD	A	591	8/8	0.89	0.23	66,69,71,71	0
3	ACY	A	596	4/4	0.89	0.22	95,95,95,96	0
4	TRS	A	600	8/8	0.92	0.20	68,70,70,71	0
3	ACY	A	595	4/4	0.92	0.17	83,83,83,83	0
3	ACY	A	603	4/4	0.94	0.12	94,94,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.