WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 11:00 PM EDT

PDB ID	:	3QJY
Title	:	Crystal structure of P-loop G234A mutant of subunit A of the A1AO ATP synthase
Authors	:	Ragunathan, P.; Manimekalai, M.S.S.; Jeyakanthan, J.; Gruber, G.
Deposited on	:	2011-01-31
Resolution	:	2.35 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

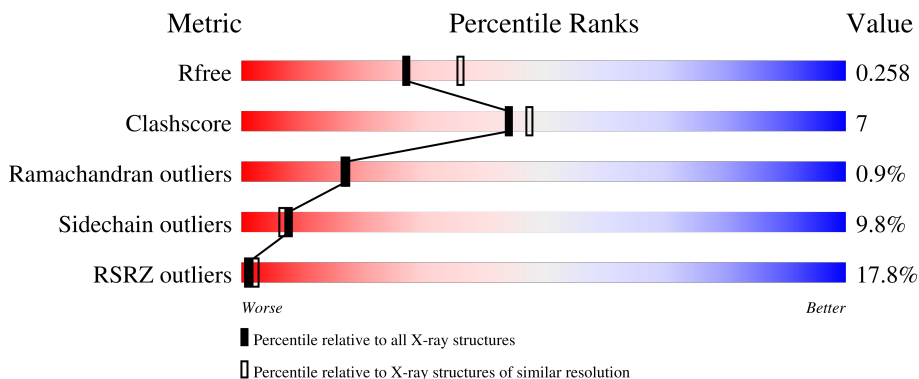|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.258
Clashscore		7
Ramachandran outliers		0.9%
Sidechain outliers		9.8%
RSRZ outliers		17.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 of 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 <=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	17% 76% 15% • 5%

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2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4650 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	556	Total 4405	C 2819	N 749	O 820	S 17	0	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ALA	GLY	engineered mutation	UNP O57728

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).
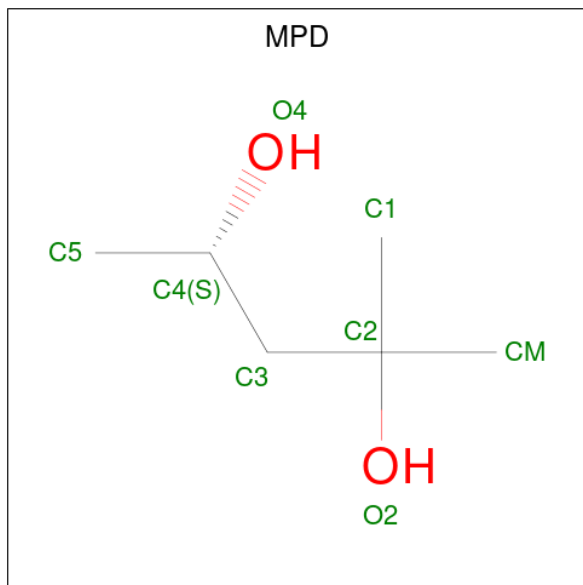
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 8	C 6	O 2	0	0
2	A	1	Total 8	C 6	O 2	0	0

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

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).
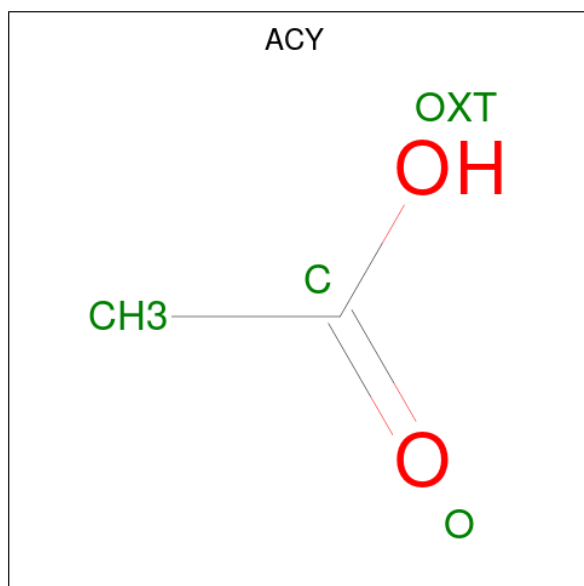
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

TRS

O2
HO
C2
C1
C
NH$_3^+$N
HO
O1
C3
OH
O3

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	201	Total	O	0	0
			201	201		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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
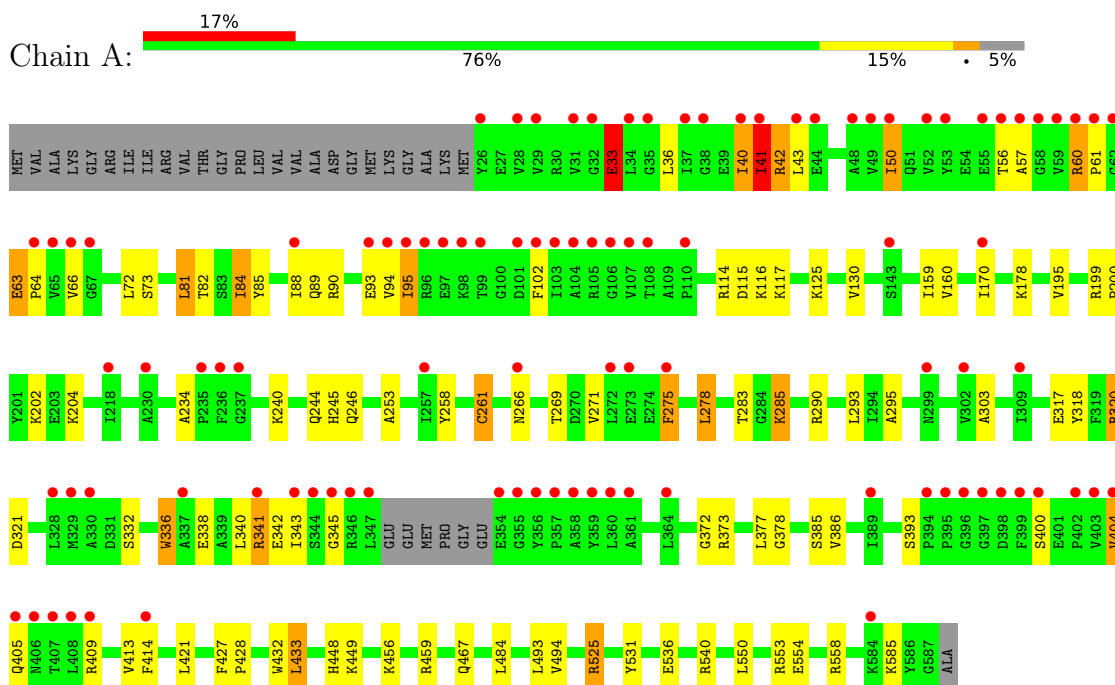
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.18Å 128.18Å 105.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.35 29.83 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.83-2.35) 99.9 (29.83-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.233 , 0.263 0.229 , 0.258	Depositor DCC
R_{free} test set	1861 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4650	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.39	0/4507	0.56	0/6105

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4405	0	4471	59	0
2	A	24	0	42	2	0
3	A	12	0	9	0	0
4	A	8	0	12	0	0
5	A	201	0	0	0	0
All	All	4650	0	4534	59	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 7.

All (59) 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:525:ARG:HH11	1:A:525:ARG:HG3	1.14	1.09
1:A:63:GLU:HB3	1:A:64:PRO:HD2	1.48	0.94
1:A:42:ARG:CG	1:A:42:ARG:HH11	1.91	0.83
1:A:199:ARG:NH2	1:A:321:ASP:OD2	2.13	0.80
1:A:525:ARG:HG3	1:A:525:ARG:NH1	1.91	0.80
1:A:261:CYS:HB3	1:A:271:VAL:HG21	1.69	0.74
1:A:40:ILE:HD13	1:A:41:ILE:H	1.53	0.73
1:A:42:ARG:HH11	1:A:42:ARG:HG2	1.55	0.72
1:A:448:HIS:HE1	1:A:456:LYS:H	1.40	0.68
1:A:525:ARG:HH11	1:A:525:ARG:CG	1.96	0.66
1:A:525:ARG:NH1	1:A:525:ARG:CG	2.58	0.63
1:A:114:ARG:HD3	1:A:170:ILE:HD11	1.81	0.61
1:A:63:GLU:HB3	1:A:64:PRO:CD	2.26	0.61
1:A:341:ARG:HH22	1:A:343:ILE:HG13	1.64	0.61
1:A:266:ASN:O	1:A:269:THR:HG22	2.02	0.60
1:A:199:ARG:NH2	1:A:318:TYR:HA	2.16	0.60
1:A:494:VAL:HG11	1:A:531:TYR:HB2	1.85	0.58
1:A:332:SER:O	1:A:336:TRP:HB3	2.04	0.57
1:A:40:ILE:HD13	1:A:41:ILE:HG13	1.87	0.57
1:A:204:LYS:HD2	1:A:372:GLY:HA3	1.86	0.57
1:A:404:VAL:HG23	1:A:405:GLN:H	1.71	0.56
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.69	0.55
1:A:373:ARG:HG3	1:A:385:SER:HB3	1.87	0.55
1:A:271:VAL:O	1:A:275:PHE:HB2	2.08	0.54
1:A:275:PHE:HA	1:A:278:LEU:HD22	1.90	0.53
1:A:130:VAL:CG1	1:A:159:ILE:HD11	2.40	0.52
1:A:253:ALA:O	1:A:290:ARG:NH2	2.42	0.51
1:A:95:ILE:O	1:A:102:PHE:HA	2.11	0.51
1:A:448:HIS:CE1	1:A:456:LYS:H	2.26	0.51
1:A:57:ALA:HB3	1:A:60:ARG:HH21	1.76	0.50
1:A:202:LYS:NZ	1:A:378:GLY:O	2.45	0.50
1:A:93:GLU:CG	1:A:94:VAL:H	2.25	0.49
1:A:317:GLU:O	1:A:320:ARG:HG3	2.13	0.49
1:A:95:ILE:HG22	1:A:102:PHE:CE1	2.50	0.47
1:A:160:VAL:HG11	1:A:178:LYS:HE3	1.97	0.46
1:A:85:TYR:HB3	1:A:89:GLN:HA	1.97	0.46
1:A:320:ARG:HG2	1:A:386:VAL:HG23	1.98	0.46
1:A:246:GLN:OE1	2:A:592:MPD:H11	2.16	0.46
1:A:200:PRO:HG2	1:A:377:LEU:HD11	1.98	0.45
1:A:130:VAL:HG11	1:A:159:ILE:HD11	1.97	0.45
1:A:400:SER:O	1:A:404:VAL:HG22	2.16	0.45
1:A:95:ILE:HG22	1:A:102:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:GLU:O	1:A:540:ARG:HG3	2.17	0.45
1:A:42:ARG:HG2	1:A:42:ARG:NH1	2.26	0.44
1:A:60:ARG:CZ	1:A:61:PRO:HD2	2.48	0.44
1:A:43:LEU:HD22	1:A:50:ILE:HD11	1.99	0.44
1:A:258:TYR:HB3	1:A:293:LEU:HD23	1.99	0.43
1:A:234:ALA:O	1:A:393:SER:HB3	2.18	0.43
1:A:33:GLU:HB3	1:A:303:ALA:HB3	2.00	0.42
1:A:93:GLU:HG3	1:A:94:VAL:H	1.85	0.42
1:A:432:TRP:CD1	1:A:433:LEU:HD13	2.55	0.42
1:A:33:GLU:HB3	1:A:303:ALA:CB	2.50	0.41
1:A:84:ILE:HD11	1:A:295:ALA:HB2	2.02	0.41
1:A:427:PHE:HA	1:A:428:PRO:C	2.40	0.41
1:A:81:LEU:O	1:A:82:THR:HB	2.21	0.41
1:A:283:THR:HB	1:A:285:LYS:HD3	2.03	0.41
1:A:554:GLU:CD	1:A:558:ARG:HH21	2.25	0.40
1:A:36:LEU:HD12	1:A:42:ARG:HD3	2.03	0.40
1:A:245[B]:HIS:CD2	2:A:592:MPD:H12	2.57	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	555/588 (94%)	504 (91%)	46 (8%)	5 (1%)	17	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	404	VAL
1	A	41	ILE
1	A	345	GLY
1	A	33	GLU

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Mol	Chain	Res	Type
1	A	63	GLU

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	472/492 (96%)	426 (90%)	46 (10%)	8	7

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	A	40	ILE
1	A	41	ILE
1	A	42	ARG
1	A	50	ILE
1	A	56	THR
1	A	60	ARG
1	A	66	VAL
1	A	72	LEU
1	A	73	SER
1	A	81	LEU
1	A	84	ILE
1	A	88	ILE
1	A	90	ARG
1	A	95	ILE
1	A	115	ASP
1	A	116	LYS
1	A	117	LYS
1	A	125	LYS
1	A	195	VAL
1	A	240	LYS
1	A	244	GLN
1	A	261	CYS
1	A	275	PHE
1	A	278	LEU

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Mol	Chain	Res	Type
1	A	285	LYS
1	A	320	ARG
1	A	336	TRP
1	A	338	GLU
1	A	340	LEU
1	A	341	ARG
1	A	342	GLU
1	A	409	ARG
1	A	413	VAL
1	A	414	PHE
1	A	421	LEU
1	A	433	LEU
1	A	449	LYS
1	A	459	ARG
1	A	467	GLN
1	A	484	LEU
1	A	493	LEU
1	A	525	ARG
1	A	550	LEU
1	A	553	ARG
1	A	585	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	A	406	ASN
1	A	448	HIS
1	A	467	GLN
1	A	504	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 (i)

There are no monosaccharides 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	592	-	7,7,7	0.29	0	9,10,10	0.34	0
3	ACY	A	590	-	3,3,3	0.74	0	3,3,3	0.88	0
2	MPD	A	589	-	7,7,7	0.28	0	9,10,10	0.27	0
4	TRS	A	591	-	7,7,7	0.28	0	9,9,9	0.17	0
2	MPD	A	593	-	7,7,7	0.29	0	9,10,10	0.34	0
3	ACY	A	594	-	3,3,3	0.78	0	3,3,3	0.85	0
3	ACY	A	595	-	3,3,3	0.76	0	3,3,3	0.88	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
4	TRS	A	591	-	-	3/9/9/9	-
2	MPD	A	589	-	-	1/5/5/5	-
2	MPD	A	592	-	-	0/5/5/5	-
2	MPD	A	593	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	589	MPD	CM-C2-C3-C4
4	A	591	TRS	C1-C-C3-O3
4	A	591	TRS	C2-C-C3-O3
4	A	591	TRS	N-C-C1-O1
2	A	593	MPD	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	592	MPD	2	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 ⓘ

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	556/588 (94%)	0.99	99 (17%)	1	2	23, 51, 129, 157	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	ILE	12.6
1	A	102	PHE	11.7
1	A	40	ILE	11.5
1	A	99	THR	11.3
1	A	343	ILE	10.6
1	A	395	PRO	10.5
1	A	65	VAL	10.0
1	A	397	GLY	9.8
1	A	396	GLY	9.2
1	A	404	VAL	8.3
1	A	405	GLN	8.0
1	A	408	LEU	7.5
1	A	38	GLY	6.9
1	A	414	PHE	6.8
1	A	66	VAL	6.7
1	A	28	VAL	6.5
1	A	29	VAL	6.5
1	A	94	VAL	6.5
1	A	97	GLU	6.5
1	A	52	VAL	6.0
1	A	49	VAL	5.8
1	A	96	ARG	5.8
1	A	98	LYS	5.8
1	A	398	ASP	5.8
1	A	403	VAL	5.8
1	A	347	LEU	5.5
1	A	361	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	59	VAL	5.4
1	A	402	PRO	5.2
1	A	357	PRO	5.1
1	A	56	THR	5.1
1	A	34	LEU	5.0
1	A	359	TYR	4.9
1	A	53	TYR	4.8
1	A	26	TYR	4.8
1	A	101	ASP	4.6
1	A	356	TYR	4.6
1	A	48	ALA	4.4
1	A	341	ARG	4.3
1	A	355	GLY	4.2
1	A	354	GLU	4.0
1	A	345	GLY	3.9
1	A	407	THR	3.8
1	A	337	ALA	3.8
1	A	43	LEU	3.8
1	A	57	ALA	3.7
1	A	67	GLY	3.6
1	A	275	PHE	3.5
1	A	58	GLY	3.5
1	A	299	ASN	3.4
1	A	64	PRO	3.4
1	A	409	ARG	3.3
1	A	406	ASN	3.3
1	A	37	ILE	3.3
1	A	236	PHE	3.3
1	A	110	PRO	3.2
1	A	266	ASN	3.2
1	A	346	ARG	3.2
1	A	61	PRO	3.1
1	A	41	ILE	3.1
1	A	399	PHE	3.1
1	A	218	ILE	3.0
1	A	235	PRO	3.0
1	A	329	MET	2.9
1	A	50	ILE	2.9
1	A	394	PRO	2.9
1	A	32	GLY	2.9
1	A	44	GLU	2.9
1	A	106	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	328	LEU	2.8
1	A	344	SER	2.8
1	A	360	LEU	2.8
1	A	55	GLU	2.8
1	A	31	VAL	2.7
1	A	103	ILE	2.7
1	A	584	LYS	2.6
1	A	389	ILE	2.6
1	A	273	GLU	2.5
1	A	272	LEU	2.5
1	A	358	ALA	2.5
1	A	107	VAL	2.4
1	A	143	SER	2.4
1	A	237	GLY	2.4
1	A	60	ARG	2.3
1	A	302	VAL	2.3
1	A	330	ALA	2.3
1	A	108	THR	2.2
1	A	400	SER	2.2
1	A	35	GLY	2.2
1	A	88	ILE	2.2
1	A	170	ILE	2.2
1	A	309	ILE	2.1
1	A	364	LEU	2.1
1	A	62	GLY	2.1
1	A	104	ALA	2.1
1	A	257	ILE	2.1
1	A	105	ARG	2.1
1	A	230	ALA	2.1
1	A	93	GLU	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	595	4/4	0.58	0.32	76,76,76,76	0
2	MPD	A	589	8/8	0.80	0.28	83,84,85,85	0
4	TRS	A	591	8/8	0.80	0.29	84,86,87,87	0
2	MPD	A	592	8/8	0.81	0.23	70,73,76,76	0
2	MPD	A	593	8/8	0.82	0.24	95,97,99,99	0
3	ACY	A	590	4/4	0.84	0.20	79,80,80,80	0
3	ACY	A	594	4/4	0.86	0.49	84,85,86,86	0

6.5 Other polymers ⓘ

There are no such residues in this entry.