



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:41 AM UTC

PDB ID : 3I72 / pdb_00003i72
Title : Structural characterization for the nucleotide binding ability of subunit A with SO4 of the A1AO ATP synthase
Authors : Manimekalai, S.M.S.; Kumar, A.; Balakrishna, A.M.; Gruber, G.
Deposited on : 2009-07-07
Resolution : 2.47 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

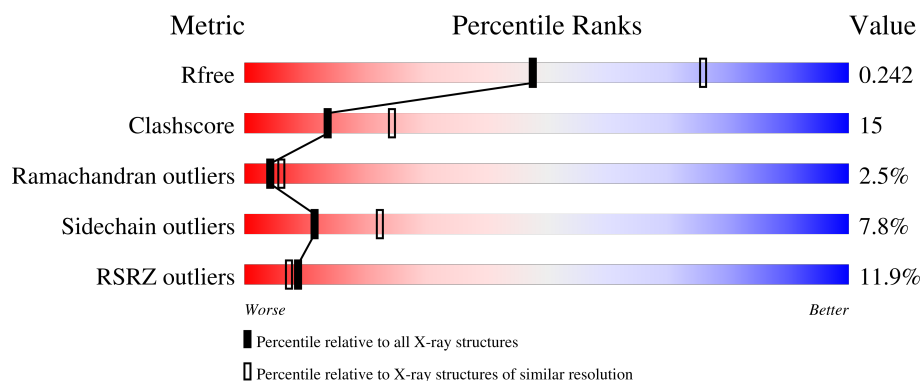
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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 $\leq 5\%$. 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
5	MPD	A	590	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MPD	A	591	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4410 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 A-TYPE ATP SYNTHASE CATALYTIC SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	514	4060	2600	691	753	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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



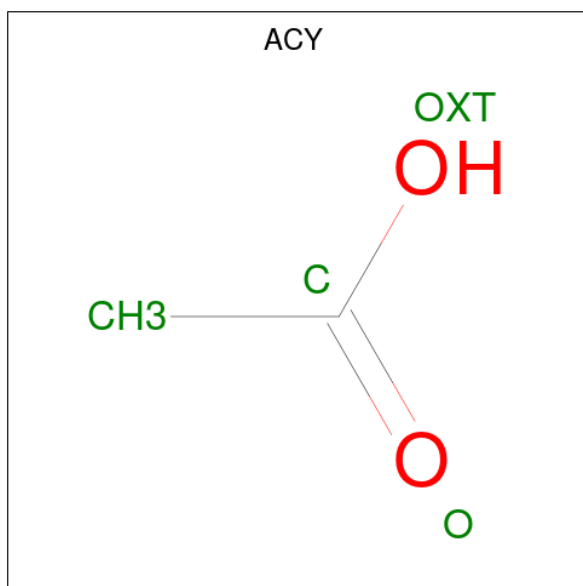
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	309	Total	O	0	0
			309	309		

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.

Chain A:

10% 63% 19% 13%

Amino Acid	Value	Amino Acid	Value	Amino Acid	Value	Amino Acid	Value		
MET	P61	VAL	H147	ALA	N296	GLY	Y381	Q505	Q505
LEU	P64	ALA	K148	LEU	S297	LEU	R382	P516	P516
GLY	V65	LEU	I159	GLY	N299	GLY	S385	V521	V521
ARG	V66	GLY	E171	ARG	M300	ARG	V386	R525	R525
ILE	V67	ILE	S181	ILE	P301	ILE	V392	L528	L528
ILE	T68	ILE	E171	ILE	A304	ILE	S393	Y531	Y531
ARG	T69	ARG	S181	ARG	R305	ARG	P394	M535	M535
VAL	S71	VAL	Q191	VAL	E306	VAL	P395	E536	E536
THR	L72	THR	Q191	THR	A307	THR	P395	A537	A537
GLY	E75	GLY	R199	GLY	S308	GLY	D398	I538	I538
PRO	P78	PRO	K202	PRO	T311	PRO	F399	M539	M539
VAL	R79	VAL	E203	VAL	I315	VAL	E401	R540	R540
VAL	S83	VAL	K204	VAL	Y318	VAL	V403	E545	E545
ASP	T84	ASP	R216	ASP	F319	ASP	V404	L550	L550
GLY	Y85	GLY	K226	GLY	R320	GLY	L408	D573	D573
LEU	D86	LEU	P233	LEU	D321	LEU	R409	E577	E577
GLY	G87	GLY	K249	GLY	L328	GLY	V410	E580	E580
ALA	T88	ALA	W250	ALA	D331	ALA	V411	K584	K584
LYS	Q89	LYS	P233	LYS	S332	LYS	L417	G587	G587
MET	R90	MET	K252	MET	T333	MET	D420	A588	A588
THR	P91	THR	D252	THR	S334	THR	L421		
GLY	E93	GLY	T257	GLY	R335	GLY	F427		
VAL	V94	VAL	Y258	VAL	W336	VAL	P428		
ARG	I95	ARG	C261	ARG	A337	ARG	L433		
VAL	E96	VAL	E262	VAL	R339	VAL	H448		
GLY	R97	GLY	E263	GLY	L340	GLY	E454		
LEU	K98	LEU	K264	LEU	ARG	LEU	W455		
GLY	T99	GLY	G265	GLY	ILE	GLY	K456		
LEU	D101	LEU	E267	LEU	SER	LEU	K457		
ILE	F102	ILE	W268	ILE	ARG	ILE	A457		
GLY	I103	GLY	W269	GLY	LEU	GLY	M458		
GLY	A104	GLY	D270	GLY	GLY	GLY	R459		
ILE	R105	ILE	V271	ILE	GLY	ILE	L465		
ILE	G106	ILE	L272	ILE	GLY	ILE	L472		
ARG	V107	ARG	E273	ARG	MET	ARG	Q473		
LEU	T108	LEU	F275	LEU	PRO	LEU	E474		
GLY	A109	GLY	P276	GLY	GLY	GLY	L484		
ASP	P110	ASP	K277	ASP	GLY	GLY	E488		
LYS	A111	LYS	L278	LYS	GLY	GLY	R489		
VAL	P113	VAL	D280	VAL	GLY	GLY	A490		
ALA	R114	ALA	P281	ALA	GLY	GLY	L493		
ILE	D115	ILE	G284	ILE	GLY	GLY	V494		
GLN	K116	GLN	K288	GLN	GLY	GLY	R499		
VAL	K117	VAL	E289	VAL	GLY	GLY			
THR	W118	THR	L293	THR	GLY	GLY			
GLY	V126	GLY		GLY	GLY	GLY			
THR	S143	THR		THR	GLY	GLY			
GLY	I144	GLY		GLY	GLY	GLY			
VAL	I145	VAL		VAL	GLY	GLY			
PRO	P146	PRO		PRO	GLY	GLY			

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.25Å 128.25Å 104.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.91 – 2.47 24.91 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.91-2.47) 99.5 (24.91-2.47)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.47Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.253 0.225 , 0.242	Depositor DCC
R_{free} test set	1597 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.9	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	0.93	EDS
Total number of atoms	4410	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 3.28% 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, TRS, MPD, SO4

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	0.79	2/4150 (0.0%)	0.99	7/5624 (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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	PRO	CA-C	6.09	1.55	1.51
1	A	199	ARG	CA-C	5.49	1.59	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ARG	N-CA-CB	5.96	119.00	110.06
1	A	108	THR	N-CA-C	5.81	123.09	114.09
1	A	410	VAL	CB-CA-C	-5.48	106.24	111.06
1	A	95	ILE	N-CA-C	5.46	120.70	109.34
1	A	394	PRO	O-C-N	5.37	123.67	121.15
1	A	199	ARG	CB-CA-C	5.20	118.25	109.67
1	A	145	ILE	N-CA-C	5.14	115.25	107.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	356	TYR	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	4060	0	4114	118	0
2	A	5	0	0	0	0
3	A	8	0	12	0	0
4	A	4	0	3	0	0
5	A	24	0	42	19	0
6	A	309	0	0	11	0
All	All	4410	0	4171	120	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 (120) 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:458:MET:HE1	1:A:525:ARG:HG2	1.13	1.09
1:A:97:GLU:HG2	1:A:98:LYS:H	1.19	1.04
1:A:458:MET:CE	1:A:525:ARG:HG2	1.96	0.96
1:A:458:MET:HE1	1:A:525:ARG:CG	1.96	0.95
1:A:433:LEU:HD22	5:A:591:MPD:HM3	1.52	0.91
1:A:249:LYS:CE	5:A:589:MPD:O2	2.20	0.90
5:A:591:MPD:HM2	6:A:688:HOH:O	1.72	0.88
1:A:249:LYS:HE2	5:A:589:MPD:O2	1.82	0.79
1:A:448:HIS:HE1	1:A:456:LYS:H	1.27	0.79
1:A:433:LEU:CD2	5:A:591:MPD:CM	2.59	0.79
1:A:216:ARG:H	1:A:505:GLN:HE22	1.30	0.78
1:A:433:LEU:HD22	5:A:591:MPD:CM	2.14	0.78
1:A:97:GLU:HG2	1:A:98:LYS:N	2.00	0.77
1:A:433:LEU:CD2	5:A:591:MPD:HM3	2.14	0.77
1:A:96:ARG:HG3	1:A:301:PRO:HD3	1.67	0.75
1:A:261:CYS:HA	1:A:296:ASN:HB2	1.69	0.75
1:A:399:PHE:HA	1:A:404:VAL:HG11	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:VAL:O	1:A:525:ARG:HG3	1.89	0.72
1:A:114:ARG:NH1	1:A:171:GLU:OE2	2.24	0.71
1:A:147:HIS:HE1	1:A:318:TYR:OH	1.74	0.70
1:A:249:LYS:NZ	5:A:589:MPD:O2	2.25	0.70
1:A:458:MET:HG2	1:A:528:LEU:HD12	1.74	0.69
1:A:373:ARG:HD2	6:A:669:HOH:O	1.92	0.68
1:A:499:ARG:NH2	6:A:649:HOH:O	2.26	0.68
1:A:528:LEU:HB3	5:A:590:MPD:C1	2.23	0.68
1:A:420:ASP:OD2	5:A:591:MPD:H51	1.93	0.67
1:A:333:THR:HG22	1:A:334:SER:H	1.59	0.66
1:A:97:GLU:HG3	1:A:105:ARG:O	1.96	0.65
1:A:528:LEU:HB3	5:A:590:MPD:H13	1.78	0.65
1:A:181:SER:HB2	6:A:746:HOH:O	1.97	0.64
1:A:257:ILE:HB	1:A:328:LEU:HD12	1.80	0.63
1:A:261:CYS:HB2	1:A:331:ASP:HB3	1.80	0.62
1:A:79:ARG:HG2	1:A:118:TRP:CZ2	2.35	0.62
1:A:263:GLU:HA	1:A:267:GLU:HB3	1.82	0.61
1:A:528:LEU:CB	5:A:590:MPD:H13	2.31	0.60
1:A:75:GLU:H	1:A:89:GLN:HE22	1.49	0.60
1:A:79:ARG:HD3	6:A:677:HOH:O	2.00	0.60
1:A:536:GLU:O	1:A:540:ARG:HG3	2.03	0.59
1:A:94:VAL:HG12	1:A:95:ILE:H	1.69	0.58
1:A:226:LYS:HE2	6:A:797:HOH:O	2.03	0.57
1:A:398:ASP:HB3	1:A:401:GLU:HG2	1.85	0.57
1:A:531:TYR:CE1	1:A:535:MET:HE3	2.39	0.57
1:A:102:PHE:HB2	1:A:103:ILE:HD12	1.87	0.56
1:A:249:LYS:HE2	5:A:589:MPD:HO2	1.70	0.56
1:A:204:LYS:HD2	1:A:372:GLY:HA3	1.87	0.56
1:A:320:ARG:HG2	1:A:386:VAL:HG23	1.88	0.55
1:A:458:MET:CE	1:A:525:ARG:HA	2.36	0.54
1:A:373:ARG:HG3	1:A:385:SER:HB3	1.88	0.54
1:A:433:LEU:CD2	5:A:591:MPD:HM1	2.35	0.54
1:A:494:VAL:HG11	1:A:531:TYR:HB2	1.89	0.54
1:A:86:ASP:OD2	1:A:90:ARG:HG2	2.08	0.53
1:A:279:LYS:HE3	1:A:284:GLY:O	2.09	0.53
1:A:100:GLY:C	1:A:102:PHE:H	2.16	0.53
1:A:143:SER:OG	1:A:289:GLU:OE2	2.25	0.53
5:A:590:MPD:H31	6:A:774:HOH:O	2.09	0.52
1:A:90:ARG:HH11	1:A:94:VAL:HG12	1.74	0.52
1:A:191:GLN:OE1	1:A:199:ARG:NH2	2.31	0.52
1:A:216:ARG:H	1:A:505:GLN:NE2	2.02	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:HIS:CE1	1:A:318:TYR:OH	2.58	0.52
1:A:79:ARG:HG2	1:A:118:TRP:CH2	2.43	0.52
1:A:458:MET:HE1	1:A:525:ARG:CB	2.39	0.52
1:A:92:LEU:O	1:A:93:GLU:HB2	2.10	0.51
1:A:458:MET:HE1	1:A:525:ARG:HA	1.91	0.51
1:A:97:GLU:CG	1:A:98:LYS:H	2.06	0.51
1:A:148:LYS:NZ	6:A:738:HOH:O	2.44	0.50
1:A:114:ARG:HH11	1:A:171:GLU:CD	2.20	0.49
1:A:333:THR:HG22	1:A:334:SER:N	2.25	0.49
1:A:433:LEU:HD23	5:A:591:MPD:HM1	1.94	0.49
1:A:580:GLU:HG2	6:A:759:HOH:O	2.14	0.47
1:A:311:THR:O	1:A:315:ILE:HG13	2.15	0.47
1:A:545:GLU:CD	1:A:545:GLU:H	2.23	0.47
1:A:458:MET:HE1	1:A:525:ARG:CA	2.45	0.47
1:A:271:VAL:CG1	1:A:293:LEU:HD21	2.45	0.46
1:A:250:TRP:CH2	1:A:281:PRO:HB2	2.50	0.46
1:A:199:ARG:HD3	1:A:321:ASP:OD2	2.16	0.46
1:A:427:PHE:HA	1:A:428:PRO:C	2.40	0.46
1:A:94:VAL:HG12	1:A:95:ILE:N	2.31	0.46
1:A:458:MET:SD	1:A:525:ARG:HG2	2.56	0.46
1:A:271:VAL:HG12	1:A:293:LEU:HD21	1.97	0.46
1:A:87:GLY:HA3	1:A:304:ALA:O	2.16	0.45
1:A:306:GLU:HG3	1:A:340:LEU:HB2	1.99	0.45
1:A:380:ASP:OD2	1:A:382:ARG:HD3	2.17	0.45
1:A:202:LYS:HE2	6:A:717:HOH:O	2.16	0.45
1:A:433:LEU:HD23	5:A:591:MPD:CM	2.45	0.45
1:A:401:GLU:HB3	1:A:402:PRO:HD2	1.98	0.44
1:A:78:PRO:O	1:A:79:ARG:HB2	2.17	0.44
1:A:87:GLY:HA2	1:A:308:SER:HB3	1.99	0.44
1:A:91:PRO:O	1:A:94:VAL:HG23	2.17	0.44
1:A:233:PRO:HA	1:A:392:VAL:O	2.17	0.44
1:A:94:VAL:CG1	1:A:95:ILE:H	2.30	0.44
1:A:116:LYS:HD3	1:A:117:LYS:N	2.33	0.44
1:A:261:CYS:H	1:A:331:ASP:HB3	1.83	0.43
1:A:96:ARG:HA	1:A:301:PRO:HG3	2.00	0.43
1:A:79:ARG:HG2	1:A:118:TRP:HZ2	1.80	0.43
1:A:79:ARG:CG	1:A:118:TRP:HZ2	2.32	0.43
1:A:88:ILE:HD11	1:A:90:ARG:HE	1.84	0.42
1:A:90:ARG:HB2	1:A:109:ALA:HB3	2.01	0.42
1:A:92:LEU:H	1:A:92:LEU:HG	1.62	0.42
1:A:484:LEU:HB3	1:A:489:ARG:HG3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:THR:OG1	1:A:100:GLY:N	2.44	0.42
1:A:459:ARG:HH11	1:A:459:ARG:HD3	1.71	0.42
1:A:126:VAL:HA	1:A:159:ILE:HG22	2.02	0.42
1:A:587:GLY:O	1:A:588:ALA:C	2.63	0.42
1:A:458:MET:HE3	5:A:590:MPD:O2	2.20	0.42
1:A:472:LEU:HD21	1:A:488:GLU:HG2	2.01	0.42
1:A:573:ASP:O	1:A:577:GLU:HG2	2.20	0.42
1:A:528:LEU:HB2	5:A:590:MPD:H13	2.03	0.41
1:A:252:ASP:OD2	6:A:702:HOH:O	2.22	0.41
1:A:338:GLU:O	1:A:338:GLU:HG3	2.21	0.41
1:A:490:ALA:HB2	1:A:538:ILE:HD12	2.02	0.41
1:A:277:LYS:HA	1:A:277:LYS:HE2	2.02	0.41
1:A:550:LEU:HD12	1:A:550:LEU:HA	1.98	0.41
1:A:339:ALA:O	1:A:340:LEU:HB3	2.21	0.41
1:A:458:MET:HE2	1:A:525:ARG:HA	2.03	0.41
1:A:258:TYR:HB3	1:A:293:LEU:HD12	2.03	0.41
1:A:531:TYR:HE1	1:A:535:MET:HE3	1.85	0.41
1:A:90:ARG:HA	1:A:91:PRO:HD3	1.84	0.40
1:A:280:ASP:HA	1:A:281:PRO:HD3	1.94	0.40
1:A:110:PRO:HB2	1:A:111:ALA:H	1.74	0.40
1:A:408:LEU:HA	1:A:411:VAL:HG22	2.04	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	510/588 (87%)	465 (91%)	32 (6%)	13 (2%)	4 6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	THR
1	A	93	GLU
1	A	110	PRO
1	A	263	GLU
1	A	357	PRO
1	A	101	ASP
1	A	334	SER
1	A	95	ILE
1	A	102	PHE
1	A	107	VAL
1	A	111	ALA
1	A	87	GLY
1	A	92	LEU

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	435/493 (88%)	401 (92%)	34 (8%)	11	22

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	83	SER
1	A	89	GLN
1	A	92	LEU
1	A	95	ILE
1	A	96	ARG
1	A	101	ASP
1	A	103	ILE
1	A	107	VAL
1	A	108	THR
1	A	116	LYS
1	A	181	SER
1	A	261	CYS
1	A	267	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	277	LYS
1	A	278	LEU
1	A	288	MET
1	A	320	ARG
1	A	328	LEU
1	A	336	TRP
1	A	363	LYS
1	A	404	VAL
1	A	417	LEU
1	A	421	LEU
1	A	433	LEU
1	A	454	GLU
1	A	459	ARG
1	A	465	LEU
1	A	474	GLU
1	A	484	LEU
1	A	493	LEU
1	A	538	ILE
1	A	577	GLU
1	A	584	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	147	HIS
1	A	426	HIS
1	A	448	HIS
1	A	450	ASN
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 ⓘ

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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	$\# Z > 2$
5	MPD	A	589	-	7,7,7	0.36	0	9,10,10	0.36	0
5	MPD	A	591	-	7,7,7	0.37	0	9,10,10	0.37	0
2	SO4	A	592	-	4,4,4	0.24	0	6,6,6	0.07	0
5	MPD	A	590	-	7,7,7	0.36	0	9,10,10	0.37	0
3	TRS	A	593	-	7,7,7	0.33	0	9,9,9	0.40	0
4	ACY	A	594	-	3,3,3	0.77	0	3,3,3	0.94	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
5	MPD	A	590	-	-	0/5/5/5	-
3	TRS	A	593	-	-	0/9/9/9	-
5	MPD	A	589	-	-	0/5/5/5	-
5	MPD	A	591	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	589	MPD	4	0
5	A	591	MPD	9	0
5	A	590	MPD	6	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	514/588 (87%)	0.48	61 (11%) 9 7	26, 50, 107, 116	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	ALA	5.6
1	A	95	ILE	5.4
1	A	99	THR	4.8
1	A	336	TRP	4.6
1	A	65	VAL	4.6
1	A	94	VAL	4.6
1	A	262	GLY	4.6
1	A	110	PRO	4.3
1	A	98	LYS	4.2
1	A	337	ALA	4.2
1	A	107	VAL	4.1
1	A	103	ILE	4.0
1	A	275	PHE	4.0
1	A	339	ALA	4.0
1	A	261	CYS	3.9
1	A	92	LEU	3.7
1	A	271	VAL	3.6
1	A	104	ALA	3.6
1	A	108	THR	3.5
1	A	100	GLY	3.5
1	A	403	VAL	3.4
1	A	357	PRO	3.4
1	A	264	ARG	3.4
1	A	102	PHE	3.2
1	A	404	VAL	3.2
1	A	270	ASP	3.1
1	A	355	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	333	THR	3.0
1	A	109	ALA	2.9
1	A	588	ALA	2.9
1	A	106	GLY	2.9
1	A	340	LEU	2.8
1	A	96	ARG	2.8
1	A	298	SER	2.7
1	A	111	ALA	2.7
1	A	72	LEU	2.7
1	A	66	VAL	2.6
1	A	338	GLU	2.6
1	A	64	PRO	2.5
1	A	68	THR	2.5
1	A	356	TYR	2.5
1	A	334	SER	2.5
1	A	268	MET	2.4
1	A	395	PRO	2.4
1	A	299	ASN	2.4
1	A	265	GLY	2.4
1	A	361	ALA	2.4
1	A	335	ARG	2.3
1	A	71	SER	2.3
1	A	272	LEU	2.3
1	A	263	GLU	2.3
1	A	278	LEU	2.2
1	A	101	ASP	2.2
1	A	93	GLU	2.2
1	A	105	ARG	2.1
1	A	400	SER	2.1
1	A	112	LEU	2.1
1	A	97	GLU	2.1
1	A	85	TYR	2.0
1	A	273	GLU	2.0
1	A	258	TYR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	MPD	A	590	8/8	0.69	0.38	10,10,10,10	0
5	MPD	A	591	8/8	0.71	0.33	10,10,10,10	0
4	ACY	A	594	4/4	0.75	0.24	91,91,92,92	0
5	MPD	A	589	8/8	0.76	0.28	10,10,10,10	0
2	SO4	A	592	5/5	0.83	0.18	87,87,88,88	0
3	TRS	A	593	8/8	0.88	0.16	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.