



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:34 PM UTC

PDB ID : 3SE0 / pdb_00003se0
Title : Structural characterization of the subunit A mutant F508W 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 : 2.62 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

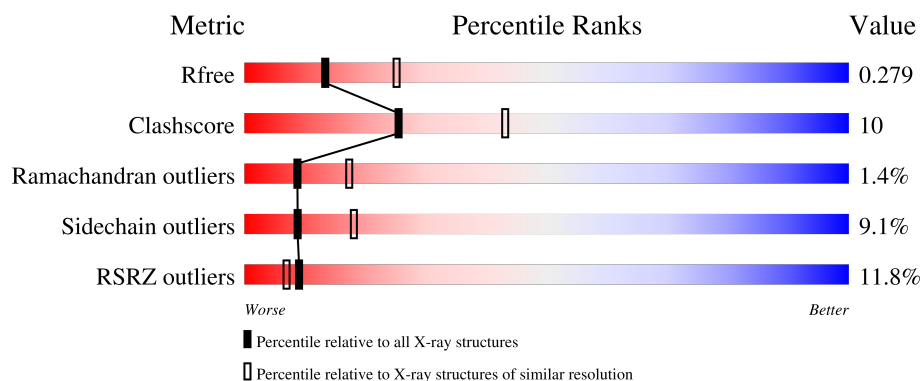
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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
4	MPD	A	594	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4297 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.

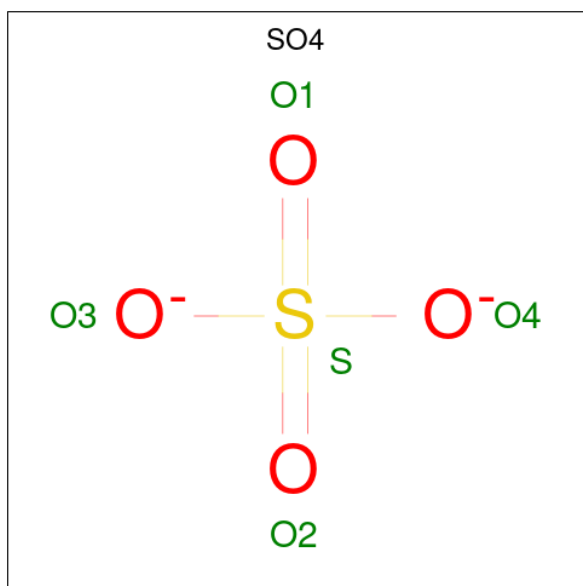
- Molecule 1 is a protein called V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	4109	2629	697	767	16	0	2	0

There is a discrepancy between the modelled and reference sequences:

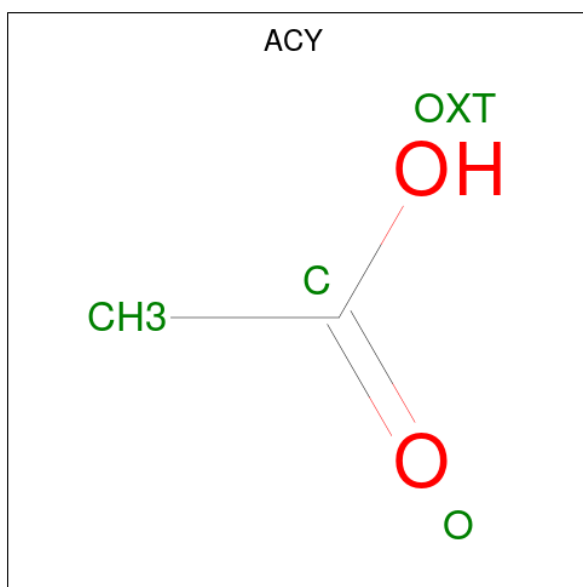
Chain	Residue	Modelled	Actual	Comment	Reference
A	508	TRP	PHE	engineered mutation	UNP O57728

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



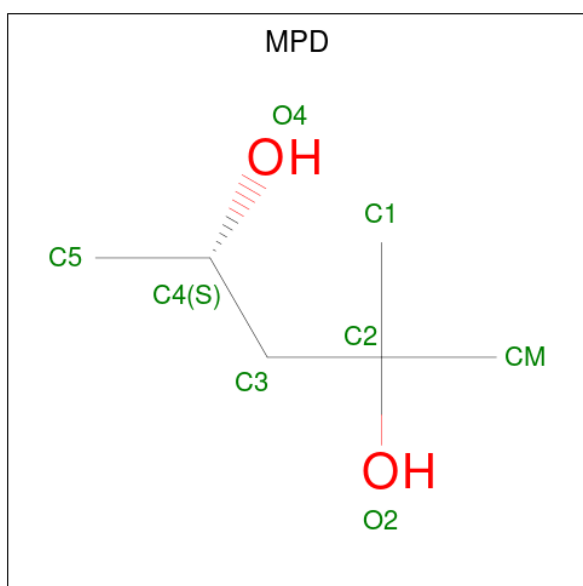
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is ACETIC ACID (CCD ID: 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		

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



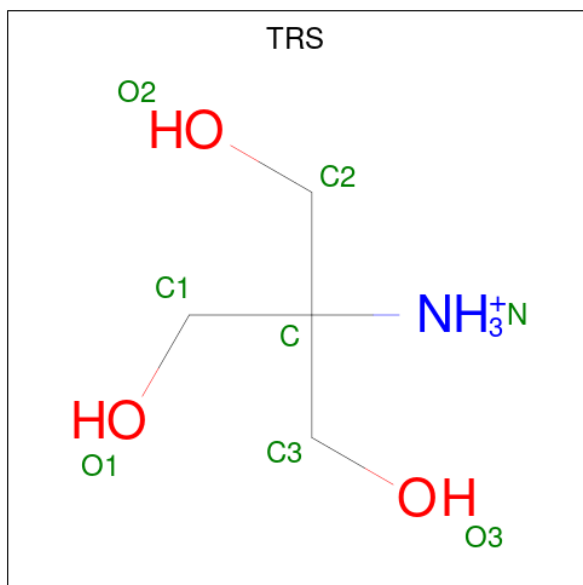
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: 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		

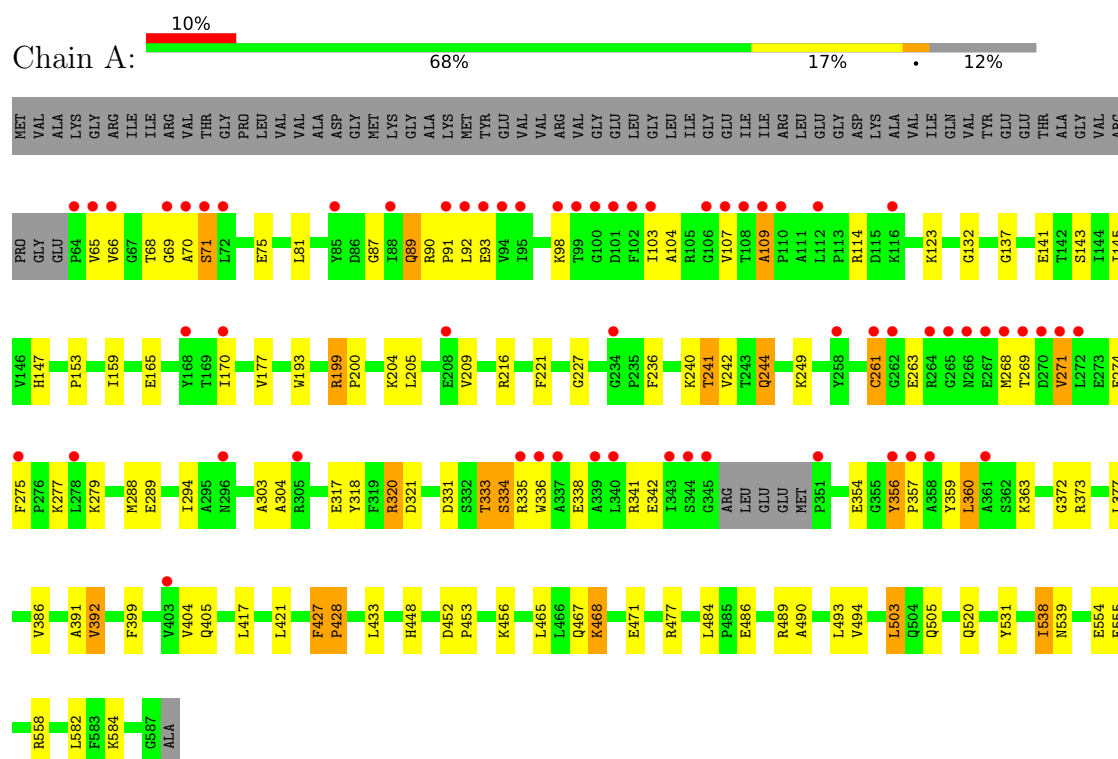
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	143	Total	O	0	0
			143	143		

3 Residue-property plots [i](#)

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	128.54Å 128.54Å 103.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.62 29.86 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.86-2.62) 99.8 (29.86-2.62)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.224 , 0.272 0.232 , 0.279	Depositor DCC
R_{free} test set	1350 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4297	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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, SO4, 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	0.62	0/4206	0.91	7/5699 (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	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	427	PHE	CA-C-N	11.45	134.15	119.84
1	A	427	PHE	C-N-CA	11.45	134.15	119.84
1	A	109	ALA	N-CA-C	6.49	118.24	110.07
1	A	427	PHE	C-N-CD	-6.26	99.34	125.00
1	A	145	ILE	N-CA-C	5.82	116.23	107.80
1	A	205	LEU	CA-C-N	-5.16	115.95	119.66
1	A	205	LEU	C-N-CA	-5.16	115.95	119.66

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	ARG	Sidechain
1	A	427	PHE	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	4109	0	4155	80	0
2	A	5	0	0	0	0
3	A	8	0	6	0	0
4	A	24	0	42	8	0
5	A	8	0	12	0	0
6	A	143	0	0	7	0
All	All	4297	0	4215	80	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 10.

All (80) 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:HG22	1:A:244:GLN:HE22	1.12	1.07
1:A:241:THR:HG22	1:A:244:GLN:NE2	1.83	0.93
1:A:68:THR:HG21	6:A:704:HOH:O	1.67	0.92
1:A:75:GLU:H	1:A:89:GLN:HE22	1.18	0.91
1:A:471:GLU:HB3	4:A:595:MPD:HM3	1.51	0.91
1:A:244:GLN:HE21	1:A:244:GLN:H	1.16	0.89
1:A:216:ARG:H	1:A:505:GLN:HE22	1.24	0.85
1:A:448:HIS:HE1	1:A:456:LYS:H	1.26	0.81
1:A:490:ALA:HB2	1:A:538:ILE:HD12	1.71	0.73
1:A:114:ARG:HE	1:A:170:ILE:HD11	1.53	0.73
1:A:199:ARG:NH1	1:A:321:ASP:OD2	2.22	0.73
1:A:490:ALA:HB2	1:A:538:ILE:CD1	2.19	0.72
1:A:249:LYS:HZ2	4:A:594:MPD:HM2	1.56	0.71
1:A:356:TYR:H	1:A:357:PRO:HD2	1.54	0.69
1:A:373:ARG:HD2	6:A:603:HOH:O	1.93	0.68
1:A:249:LYS:NZ	4:A:594:MPD:HM2	2.08	0.68
1:A:241:THR:CG2	1:A:244:GLN:HE22	2.00	0.66
1:A:75:GLU:H	1:A:89:GLN:NE2	1.93	0.65
1:A:341:ARG:CG	1:A:342:GLU:H	2.08	0.65
1:A:320:ARG:HG2	1:A:386:VAL:HG23	1.77	0.65
1:A:341:ARG:HG3	1:A:342:GLU:N	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:HIS:CE1	1:A:456:LYS:H	2.12	0.64
1:A:199:ARG:HH11	1:A:318:TYR:HA	1.61	0.63
1:A:204:LYS:HD2	1:A:372:GLY:HA3	1.79	0.63
1:A:216:ARG:H	1:A:505:GLN:NE2	1.94	0.63
1:A:147:HIS:HE1	1:A:318:TYR:OH	1.84	0.61
1:A:341:ARG:HG3	1:A:342:GLU:H	1.66	0.59
1:A:428:PRO:HB2	6:A:620:HOH:O	2.03	0.59
1:A:554:GLU:OE2	1:A:558:ARG:NH2	2.31	0.58
1:A:242:VAL:HB	4:A:594:MPD:H13	1.85	0.57
1:A:98:LYS:HE2	1:A:303:ALA:HB1	1.87	0.57
1:A:104:ALA:HB2	6:A:729:HOH:O	2.04	0.57
1:A:494:VAL:HG11	1:A:531:TYR:HB2	1.87	0.56
1:A:275:PHE:HE1	6:A:736:HOH:O	1.89	0.55
1:A:360:LEU:H	1:A:360:LEU:HD13	1.72	0.55
1:A:141:GLU:OE1	1:A:147:HIS:HD2	1.90	0.55
1:A:341:ARG:CG	1:A:342:GLU:N	2.71	0.54
1:A:317:GLU:O	1:A:320:ARG:HG3	2.08	0.54
1:A:467:GLN:NE2	6:A:629:HOH:O	2.30	0.54
1:A:199:ARG:NH1	1:A:318:TYR:HA	2.23	0.53
1:A:153:PRO:HG2	1:A:193:TRP:CZ3	2.44	0.52
1:A:143:SER:OG	1:A:289:GLU:OE2	2.27	0.52
1:A:249:LYS:NZ	4:A:594:MPD:CM	2.74	0.51
1:A:244:GLN:NE2	1:A:244:GLN:H	1.97	0.51
1:A:68:THR:HG22	1:A:69:GLY:N	2.26	0.50
1:A:333:THR:C	1:A:335:ARG:H	2.20	0.50
1:A:236:PHE:CE2	1:A:391:ALA:HB2	2.47	0.49
1:A:490:ALA:CB	1:A:538:ILE:HD12	2.40	0.49
1:A:399:PHE:C	1:A:404:VAL:HG21	2.38	0.48
1:A:356:TYR:H	1:A:357:PRO:CD	2.22	0.48
1:A:65:VAL:HB	1:A:359:TYR:CE1	2.48	0.48
1:A:249:LYS:CE	4:A:594:MPD:H4	2.44	0.47
1:A:123:LYS:HG2	1:A:137:GLY:HA2	1.97	0.47
1:A:261:CYS:HB3	1:A:331:ASP:HB3	1.97	0.47
1:A:271:VAL:HB	1:A:274:GLU:HB2	1.96	0.46
1:A:91:PRO:HD2	1:A:109:ALA:HB3	1.98	0.46
1:A:70:ALA:HB3	1:A:103:ILE:HG12	1.98	0.46
1:A:159:ILE:HD13	1:A:177:VAL:HG22	1.98	0.45
1:A:275:PHE:HB3	1:A:288:MET:HE2	1.99	0.45
1:A:468:LYS:HE3	1:A:468:LYS:HA	1.99	0.44
1:A:392:VAL:HG13	1:A:404:VAL:HG12	2.00	0.44
1:A:123:LYS:HD3	1:A:123:LYS:HA	1.68	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLN:HE21	1:A:244:GLN:N	1.99	0.44
1:A:200:PRO:HG2	1:A:377:LEU:HD11	2.00	0.43
1:A:452:ASP:HA	1:A:453:PRO:HD3	1.87	0.43
1:A:87:GLY:HA3	1:A:304:ALA:O	2.19	0.42
1:A:132:GLY:O	1:A:377:LEU:HB3	2.19	0.42
1:A:241:THR:HG23	6:A:654:HOH:O	2.19	0.42
1:A:249:LYS:HZ1	4:A:594:MPD:CM	2.33	0.42
1:A:275:PHE:C	1:A:277:LYS:H	2.28	0.41
1:A:486:GLU:OE2	1:A:489:ARG:NH1	2.53	0.41
1:A:65:VAL:HB	1:A:359:TYR:CZ	2.56	0.41
1:A:216:ARG:N	1:A:505:GLN:HE22	2.04	0.41
1:A:221:PHE:CE1	1:A:503:LEU:HD11	2.56	0.41
1:A:242:VAL:HB	4:A:594:MPD:C1	2.51	0.41
1:A:399:PHE:HA	1:A:404:VAL:HG11	2.03	0.41
1:A:216:ARG:HG2	1:A:520:GLN:HG2	2.03	0.41
1:A:271:VAL:HG23	1:A:275:PHE:CD2	2.56	0.41
1:A:227:GLY:HA2	1:A:386:VAL:O	2.21	0.40
1:A:90:ARG:HA	1:A:91:PRO:HD3	1.93	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	517/588 (88%)	479 (93%)	31 (6%)	7 (1%)	9 17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	VAL
1	A	334	SER
1	A	428	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	356	TYR
1	A	71	SER
1	A	107	VAL
1	A	336	TRP

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	441/492 (90%)	401 (91%)	40 (9%)	9 18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	71	SER
1	A	81	LEU
1	A	89	GLN
1	A	92	LEU
1	A	93	GLU
1	A	165	GLU
1	A	209	VAL
1	A	240	LYS
1	A	241	THR
1	A	244	GLN
1	A	261	CYS
1	A	263	GLU
1	A	268	MET
1	A	269	THR
1	A	279	LYS
1	A	294	ILE
1	A	320	ARG
1	A	333	THR
1	A	334	SER
1	A	338	GLU
1	A	354	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	360	LEU
1	A	363	LYS
1	A	392	VAL
1	A	405	GLN
1	A	417	LEU
1	A	421	LEU
1	A	433	LEU
1	A	465	LEU
1	A	468	LYS
1	A	477	ARG
1	A	484	LEU
1	A	493	LEU
1	A	503	LEU
1	A	538	ILE
1	A	539	ASN
1	A	555	GLU
1	A	582	LEU
1	A	584	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	147	HIS
1	A	215	GLN
1	A	224	GLN
1	A	244	GLN
1	A	296	ASN
1	A	448	HIS
1	A	450	ASN
1	A	467	GLN
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 oligosaccharides 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	$\# Z > 2$
4	MPD	A	594	-	7,7,7	0.33	0	9,10,10	0.49	0
4	MPD	A	591	-	7,7,7	0.34	0	9,10,10	0.48	0
2	SO4	A	589	-	4,4,4	0.24	0	6,6,6	0.11	0
4	MPD	A	595	-	7,7,7	0.34	0	9,10,10	0.49	0
3	ACY	A	590	-	3,3,3	0.79	0	3,3,3	0.85	0
5	TRS	A	592	-	7,7,7	0.33	0	9,9,9	0.41	0
3	ACY	A	593	-	3,3,3	0.84	0	3,3,3	0.69	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	MPD	A	594	-	-	1/5/5/5	-
5	TRS	A	592	-	-	5/9/9/9	-
4	MPD	A	595	-	-	1/5/5/5	-
4	MPD	A	591	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	592	TRS	C2-C-C3-O3
5	A	592	TRS	N-C-C3-O3
4	A	591	MPD	O2-C2-C3-C4
4	A	594	MPD	O2-C2-C3-C4
4	A	595	MPD	O2-C2-C3-C4
5	A	592	TRS	C1-C-C3-O3
5	A	592	TRS	C3-C-C2-O2
5	A	592	TRS	N-C-C2-O2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	594	MPD	7	0
4	A	595	MPD	1	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	519/588 (88%)	0.51	61 (11%) 9 7	23, 57, 130, 186	2 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	ILE	5.8
1	A	94	VAL	5.5
1	A	103	ILE	5.4
1	A	92	LEU	5.4
1	A	70	ALA	5.3
1	A	107	VAL	5.1
1	A	272	LEU	4.9
1	A	340	LEU	4.6
1	A	337	ALA	4.4
1	A	98	LYS	4.1
1	A	65	VAL	3.9
1	A	100	GLY	3.9
1	A	66	VAL	3.8
1	A	335	ARG	3.7
1	A	336	TRP	3.5
1	A	343	ILE	3.5
1	A	269	THR	3.5
1	A	339	ALA	3.4
1	A	345	GLY	3.4
1	A	271	VAL	3.4
1	A	234	GLY	3.3
1	A	170	ILE	3.2
1	A	268	MET	3.2
1	A	356	TYR	3.2
1	A	93	GLU	3.1
1	A	270	ASP	3.1
1	A	261	CYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	71	SER	3.0
1	A	106	GLY	2.9
1	A	101	ASP	2.8
1	A	109	ALA	2.8
1	A	108	THR	2.8
1	A	403	VAL	2.8
1	A	112	LEU	2.8
1	A	262	GLY	2.7
1	A	265	GLY	2.7
1	A	357	PRO	2.7
1	A	275	PHE	2.6
1	A	102	PHE	2.6
1	A	99	THR	2.6
1	A	168	TYR	2.5
1	A	358	ALA	2.5
1	A	208	GLU	2.4
1	A	264	ARG	2.4
1	A	91	PRO	2.4
1	A	110	PRO	2.4
1	A	72	LEU	2.3
1	A	64	PRO	2.3
1	A	344	SER	2.3
1	A	116	LYS	2.2
1	A	266	ASN	2.2
1	A	85	TYR	2.2
1	A	305	ARG	2.2
1	A	278	LEU	2.1
1	A	351	PRO	2.1
1	A	88	ILE	2.1
1	A	267	GLU	2.1
1	A	361	ALA	2.1
1	A	258	TYR	2.1
1	A	296	ASN	2.0
1	A	69	GLY	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
3	ACY	A	590	4/4	0.59	0.25	93,93,93,94	0
4	MPD	A	591	8/8	0.78	0.16	84,85,86,86	0
3	ACY	A	593	4/4	0.82	0.24	80,80,80,81	0
4	MPD	A	595	8/8	0.83	0.25	84,85,86,86	0
5	TRS	A	592	8/8	0.88	0.20	96,97,97,97	0
4	MPD	A	594	8/8	0.89	0.25	84,85,86,86	0
2	SO4	A	589	5/5	0.91	0.18	106,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.