



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:13 AM UTC

PDB ID : 3SDZ / pdb_00003sdz
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 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

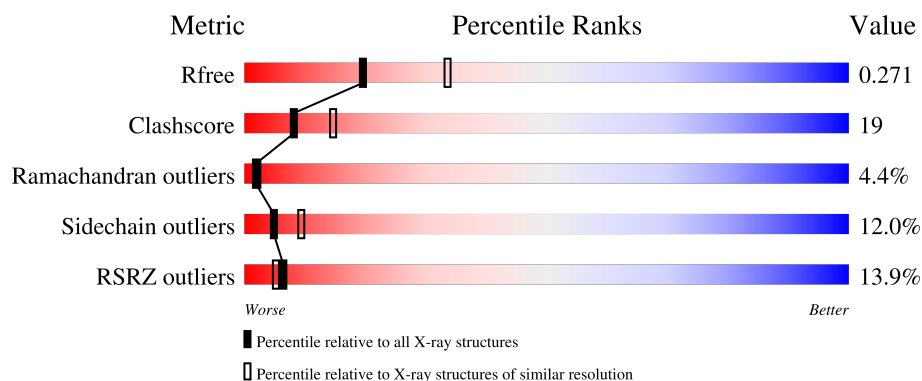
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (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 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	

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.

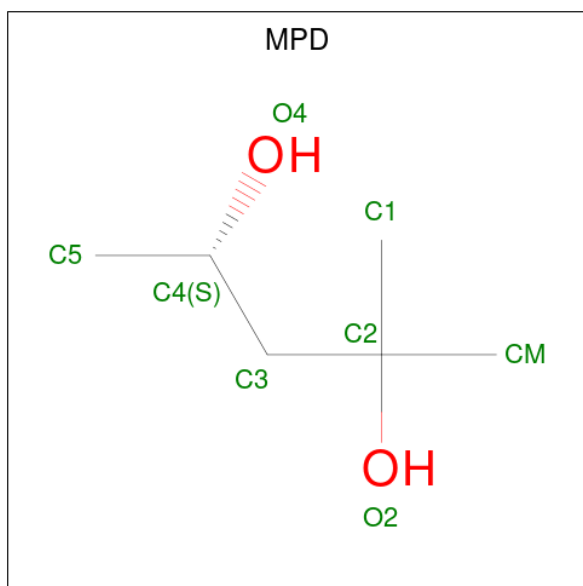
- Molecule 1 is a protein called V-type ATP synthase alpha chain.

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

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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



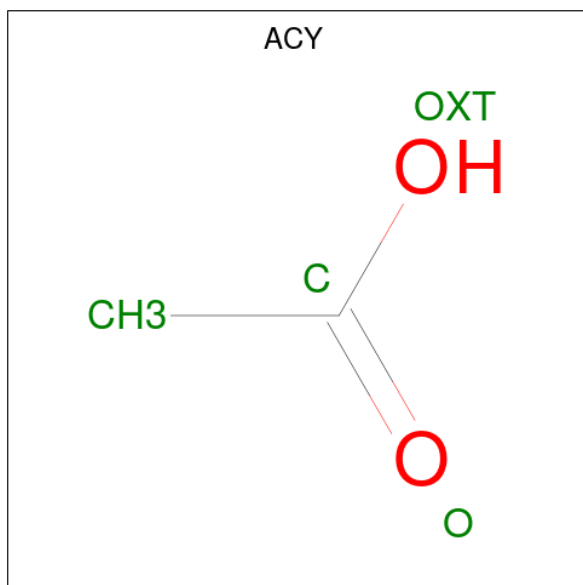
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		

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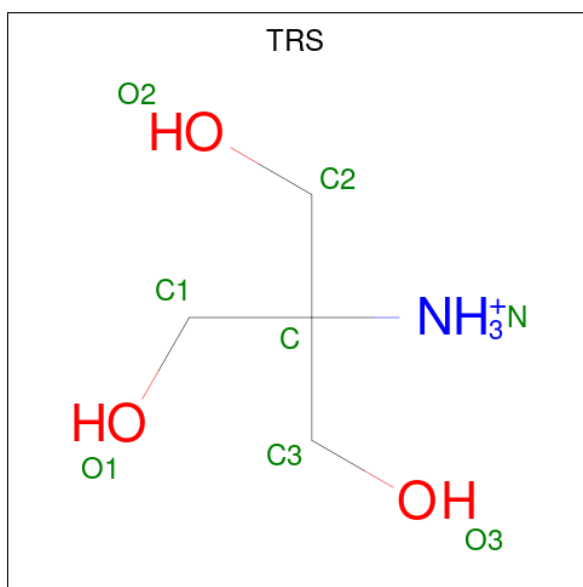
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		

- 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		
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 (CCD ID: 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		

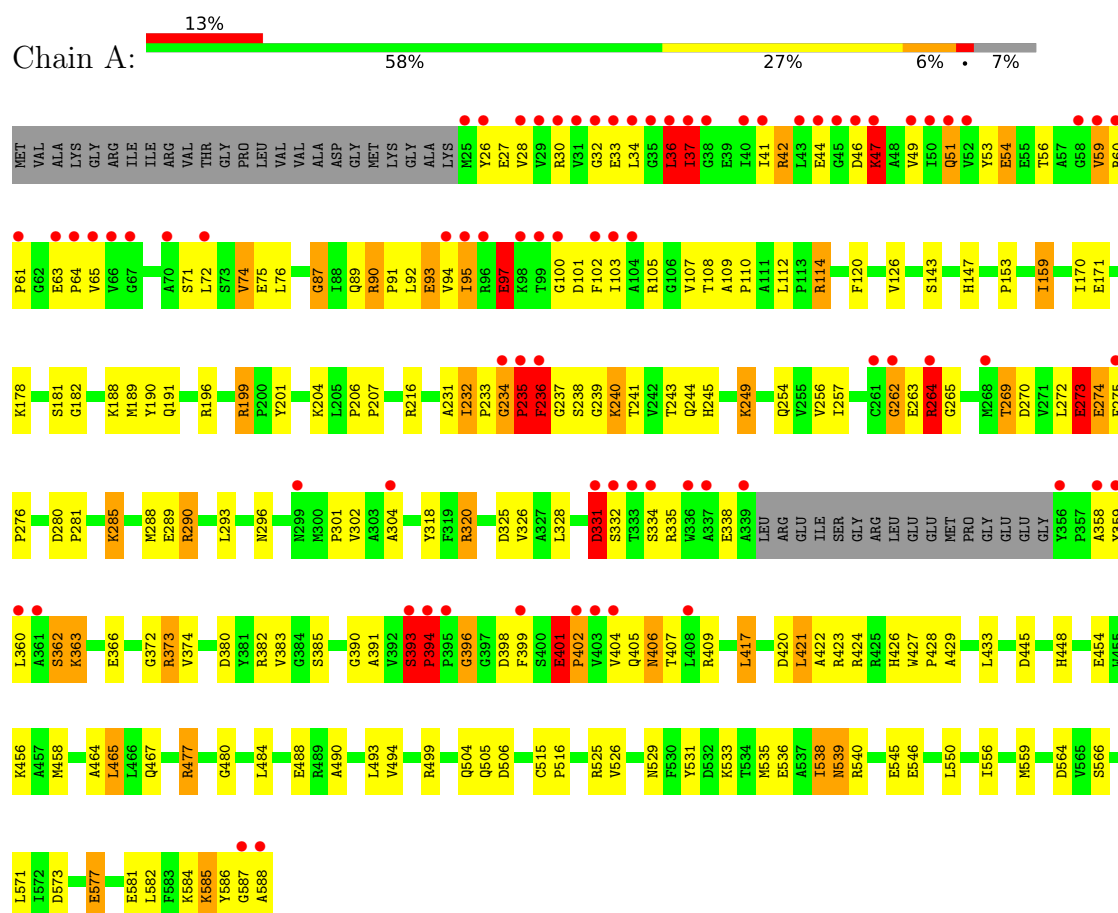
- Molecule 5 is water.

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

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	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 (5.07%)	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 , 59.9	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	1.15	4/4431 (0.1%)	1.25	24/6005 (0.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	429	ALA	CA-CB	7.10	1.62	1.52
1	A	37	ILE	CA-CB	6.95	1.64	1.54
1	A	516	PRO	CA-C	5.72	1.55	1.51
1	A	422	ALA	CA-CB	-5.04	1.45	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	SER	CA-C-N	12.98	133.75	120.38
1	A	393	SER	C-N-CA	12.98	133.75	120.38
1	A	394	PRO	N-CA-C	7.75	120.16	110.70
1	A	407	THR	N-CA-C	-7.29	103.33	111.71
1	A	515	CYS	CA-C-N	-7.20	114.41	119.66
1	A	515	CYS	C-N-CA	-7.20	114.41	119.66
1	A	90	ARG	CA-C-N	6.87	126.85	119.78
1	A	90	ARG	C-N-CA	6.87	126.85	119.78
1	A	59	VAL	N-CA-C	6.71	123.29	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	LEU	CA-C-N	-6.56	112.94	119.56
1	A	550	LEU	C-N-CA	-6.56	112.94	119.56
1	A	373	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	A	87	GLY	N-CA-C	6.46	121.57	114.40
1	A	334	SER	N-CA-C	6.45	120.34	109.76
1	A	36	LEU	N-CA-C	6.42	119.60	109.96
1	A	199	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	A	373	ARG	CG-CD-NE	-6.10	98.58	112.00
1	A	332	SER	N-CA-C	5.82	117.84	110.33
1	A	182	GLY	N-CA-C	-5.66	107.21	114.85
1	A	42	ARG	N-CA-C	5.60	118.46	111.24
1	A	480	GLY	CA-C-N	5.53	126.39	120.47
1	A	480	GLY	C-N-CA	5.53	126.39	120.47
1	A	320	ARG	N-CA-CB	5.30	117.91	110.12
1	A	362	SER	N-CA-C	-5.18	105.71	112.23

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	161	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	173	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 19.

All (173) 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:526:VAL:HG11	1:A:559:MET:HE1	1.26	1.11
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:559:MET:HE2	1:A:571:LEU:HD12	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:406:ASN:HB3	1:A:409:ARG:HB2	1.62	0.82
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: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:584:LYS:C	1:A:586:TYR:H	1.99	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
1:A:120:PHE:HB2	1:A:189:MET:HE3	1.74	0.69
2:A:589:MPD:H11	2:A:589:MPD:O4	1.92	0.69
1:A:494:VAL:HG11	1:A:531:TYR:HB2	1.73	0.69
2:A:590:MPD:O4	2:A:590:MPD:H11	1.92	0.69
1:A:273:GLU:HA	1:A:276:PRO:HD2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:HIS:HE1	1:A:456:LYS:H	1.42	0.67
1:A:556:ILE:HA	1:A:559:MET:HE3	1.77	0.66
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:O4	2:A:602:MPD:HM1	1.96	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:74:VAL:HG11	1:A:76:LEU:HD21	1.79	0.63
1:A:262:GLY:HA3	1:A:296:ASN:O	1.99	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
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:H11	2:A:594:MPD:O4	2.06	0.56
1:A:61:PRO:HD2	1:A:65:VAL:HG23	1.87	0.55
1:A:254:GLN:HE22	1:A:325:ASP:H	1.54	0.55
1:A:360:LEU:C	1:A:362:SER:H	2.13	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:O4	2:A:590:MPD:C1	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:VAL:CG1	1:A:559:MET:HE1	2.18	0.55
1:A:153:PRO:HD3	1:A:191:GLN:HE22	1.71	0.55
1:A:526:VAL:HG11	1:A:559:MET:CE	2.18	0.54
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:584:LYS:C	1:A:586:TYR:N	2.66	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:559:MET:HE2	1:A:571:LEU:CD1	2.32	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:427:TRP:HA	1:A:428:PRO:C	2.34	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:O4	2:A:591:MPD:C1	2.58	0.51
1:A:426:HIS:HE1	5:A:612:HOH:O	1.92	0.51
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
1:A:394:PRO:C	1:A:396:GLY:H	2.20	0.50
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: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: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:216:ARG:N	1:A:505:GLN:HE22	2.02	0.46
1:A:236:PHE:CB	5:A:860:HOH:O	2.63	0.46
1:A:206:PRO:O	1:A:207:PRO:C	2.55	0.46
1:A:288:MET:HE1	1:A:293:LEU:HG	1.98	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:458:MET:HE1	1:A:525:ARG:HB2	1.97	0.46
1:A:236:PHE:HB2	5:A:860:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:MET:O	1:A:539:ASN:HB2	2.16	0.45
1:A:564:ASP:OD1	1:A:566:SER:OG	2.33	0.45
1:A:249:LYS:HZ1	1:A:281:PRO:HG3	1.82	0.45
1:A:95:ILE:HB	1:A:103:ILE:O	2.17	0.45
1:A:394:PRO:C	1:A:396:GLY:N	2.75	0.45
1:A:402:PRO:O	1:A:405:GLN:HB3	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:264:ARG:CG	1:A:265:GLY:N	2.68	0.44
1:A:53:TYR:CE2	1:A:56:THR:HA	2.53	0.44
1:A:275:PHE:N	1:A:276:PRO:CD	2.81	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:33:GLU:C	1:A:34:LEU:HG	2.43	0.43
1:A:421:LEU:HD12	1:A:421:LEU:HA	1.87	0.43
1:A:360:LEU:C	1:A:362:SER:N	2.77	0.43
1:A:72:LEU:HD12	5:A:819:HOH:O	2.18	0.43
1:A:404:VAL:O	1:A:405:GLN:C	2.61	0.43
1:A:236:PHE:CE2	1:A:238:SER:HB2	2.54	0.43
1:A:581:GLU:HA	1:A:584:LYS:HZ2	1.82	0.43
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:237:GLY:C	1:A:239:GLY:N	2.77	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:75:GLU:CD	1:A:114:ARG:HH22	2.27	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:171:GLU:O	1:A:188:LYS:HE2	2.20	0.42
1:A:577[A]:GLU:HG2	1:A:577[A]:GLU:H	1.56	0.41
1:A:285:LYS:H	1:A:285:LYS:HG2	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ARG:O	1:A:504:GLN:HG3	2.20	0.41
1:A:90:ARG:HA	1:A:91:PRO:HD3	1.87	0.41
4:A:601:TRS:O2	4:A:601:TRS:O1	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:231:ALA:HA	1:A:390:GLY:O	2.21	0.41
1:A:273:GLU:HA	1:A:276:PRO:HG2	2.02	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: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
1:A:545:GLU:H	1:A:545:GLU:CD	2.29	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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Mol	Chain	Res	Type
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%)	406 (88%)	56 (12%)	5 9

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	TYR
1	A	30	ARG
1	A	36	LEU
1	A	37	ILE
1	A	41	ILE

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Mol	Chain	Res	Type
1	A	47	LYS
1	A	49	VAL
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	232	ILE
1	A	236	PHE
1	A	240	LYS
1	A	243	THR
1	A	249	LYS
1	A	264	ARG
1	A	269	THR
1	A	272	LEU
1	A	273	GLU
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	338	GLU
1	A	359	TYR
1	A	363	LYS
1	A	393	SER
1	A	417	LEU
1	A	421	LEU
1	A	433	LEU
1	A	445	ASP
1	A	454	GLU

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Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	147	HIS
1	A	191	GLN
1	A	224	GLN
1	A	254	GLN
1	A	426	HIS
1	A	448	HIS
1	A	450	ASN
1	A	504	GLN
1	A	505	GLN
1	A	529	ASN
1	A	576	ASN

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

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	589	-	7,7,7	3.10	1 (14%)	9,10,10	3.49	3 (33%)
3	ACY	A	596	-	3,3,3	0.78	0	3,3,3	0.80	0
2	MPD	A	591	-	7,7,7	0.32	0	9,10,10	0.21	0
3	ACY	A	593	-	3,3,3	0.76	0	3,3,3	1.18	0
2	MPD	A	594	-	7,7,7	0.31	0	9,10,10	0.22	0
2	MPD	A	592	-	7,7,7	3.10	1 (14%)	9,10,10	3.49	3 (33%)
3	ACY	A	595	-	3,3,3	0.73	0	3,3,3	1.00	0
3	ACY	A	603	-	3,3,3	0.82	0	3,3,3	0.76	0
2	MPD	A	602	-	7,7,7	1.30	2 (28%)	9,10,10	0.21	0
4	TRS	A	600	-	7,7,7	0.47	0	9,9,9	0.93	0
2	MPD	A	590	-	7,7,7	3.10	1 (14%)	9,10,10	3.49	3 (33%)
3	ACY	A	597	-	3,3,3	0.84	0	3,3,3	0.74	0
4	TRS	A	601	-	7,7,7	0.49	0	9,9,9	1.39	2 (22%)
3	ACY	A	598	-	3,3,3	0.79	0	3,3,3	0.93	0
4	TRS	A	599	-	7,7,7	0.35	0	9,9,9	0.84	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
2	MPD	A	589	-	-	1/5/5/5	-
2	MPD	A	591	-	-	1/5/5/5	-
2	MPD	A	594	-	-	1/5/5/5	-
2	MPD	A	592	-	-	1/5/5/5	-
2	MPD	A	602	-	-	0/5/5/5	-
4	TRS	A	600	-	-	7/9/9/9	-
2	MPD	A	590	-	-	1/5/5/5	-
4	TRS	A	601	-	-	7/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	A	599	-	-	6/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	590	MPD	O4-C4	-8.07	1.10	1.43
2	A	589	MPD	O4-C4	-8.06	1.10	1.43
2	A	592	MPD	O4-C4	-8.06	1.10	1.43
2	A	602	MPD	C5-C4	-2.41	1.41	1.51
2	A	602	MPD	O4-C4	2.37	1.52	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	589	MPD	O4-C4-C3	-9.22	74.65	111.35
2	A	592	MPD	O4-C4-C3	-9.22	74.67	111.35
2	A	590	MPD	O4-C4-C3	-9.21	74.70	111.35
2	A	589	MPD	C5-C4-C3	3.63	128.52	111.67
2	A	590	MPD	C5-C4-C3	3.62	128.49	111.67
2	A	592	MPD	C5-C4-C3	3.62	128.48	111.67
4	A	601	TRS	O3-C3-C	2.37	117.48	110.88
2	A	589	MPD	O2-C2-CM	-2.21	101.09	107.99
2	A	592	MPD	O2-C2-CM	-2.21	101.09	107.99
2	A	590	MPD	O2-C2-CM	-2.21	101.09	107.99
4	A	601	TRS	O2-C2-C	-2.01	105.26	110.88

There are no chirality outliers.

All (25) 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
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	600	TRS	N-C-C1-O1
4	A	600	TRS	N-C-C3-O3
4	A	601	TRS	C2-C-C1-O1
4	A	601	TRS	N-C-C1-O1

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Mol	Chain	Res	Type	Atoms
4	A	601	TRS	C3-C-C2-O2
2	A	591	MPD	O2-C2-C3-C4
2	A	594	MPD	O2-C2-C3-C4
4	A	599	TRS	C1-C-C2-O2
4	A	600	TRS	C3-C-C1-O1
4	A	600	TRS	C1-C-C3-O3
4	A	601	TRS	C3-C-C1-O1
4	A	599	TRS	C3-C-C2-O2
4	A	600	TRS	N-C-C2-O2
4	A	600	TRS	C2-C-C3-O3
2	A	589	MPD	C1-C2-C3-C4
2	A	590	MPD	C1-C2-C3-C4
2	A	592	MPD	C1-C2-C3-C4
4	A	601	TRS	N-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	589	MPD	4	0
2	A	591	MPD	3	0
2	A	594	MPD	1	0
2	A	592	MPD	5	0
2	A	602	MPD	1	0
2	A	590	MPD	2	0
4	A	601	TRS	1	0
3	A	598	ACY	1	0
4	A	599	TRS	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	548/588 (93%)	0.39	76 (13%) 6 5	22, 51, 126, 165	2 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ILE	8.5
1	A	49	VAL	6.4
1	A	59	VAL	6.4
1	A	95	ILE	5.3
1	A	50	ILE	4.8
1	A	61	PRO	4.7
1	A	64	PRO	4.5
1	A	99	THR	4.4
1	A	588	ALA	4.3
1	A	66	VAL	4.1
1	A	29	VAL	4.0
1	A	35	GLY	3.9
1	A	51	GLN	3.8
1	A	356	TYR	3.7
1	A	337	ALA	3.6
1	A	41	ILE	3.5
1	A	31	VAL	3.5
1	A	402	PRO	3.5
1	A	44	GLU	3.4
1	A	43	LEU	3.4
1	A	339	ALA	3.4
1	A	234	GLY	3.4
1	A	403	VAL	3.3
1	A	358	ALA	3.3
1	A	235	PRO	3.3
1	A	46	ASP	3.2
1	A	40	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	393	SER	3.1
1	A	394	PRO	3.1
1	A	45	GLY	3.0
1	A	65	VAL	2.9
1	A	60	ARG	2.9
1	A	36	LEU	2.9
1	A	399	PHE	2.9
1	A	264	ARG	2.8
1	A	103	ILE	2.7
1	A	28	VAL	2.7
1	A	268	MET	2.7
1	A	275	PHE	2.7
1	A	334	SER	2.7
1	A	102	PHE	2.7
1	A	98	LYS	2.6
1	A	52	VAL	2.6
1	A	30	ARG	2.6
1	A	236	PHE	2.6
1	A	404	VAL	2.6
1	A	58	GLY	2.6
1	A	47	LYS	2.6
1	A	359	TYR	2.6
1	A	26	TYR	2.5
1	A	38	GLY	2.5
1	A	32	GLY	2.4
1	A	63	GLU	2.4
1	A	587	GLY	2.4
1	A	261	CYS	2.4
1	A	96	ARG	2.4
1	A	332	SER	2.4
1	A	361	ALA	2.4
1	A	94	VAL	2.3
1	A	100	GLY	2.3
1	A	333	THR	2.3
1	A	25	MET	2.2
1	A	331	ASP	2.2
1	A	299	ASN	2.2
1	A	304	ALA	2.2
1	A	34	LEU	2.2
1	A	33	GLU	2.2
1	A	336	TRP	2.2
1	A	72	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	408	LEU	2.2
1	A	67	GLY	2.1
1	A	262	GLY	2.1
1	A	395	PRO	2.1
1	A	104	ALA	2.1
1	A	70	ALA	2.0
1	A	360	LEU	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 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(Å ²)	Q<0.9
3	ACY	A	597	4/4	0.58	0.22	121,121,121,121	0
2	MPD	A	594	8/8	0.70	0.24	88,90,91,92	0
4	TRS	A	599	8/8	0.74	0.17	86,88,89,89	0
3	ACY	A	598	4/4	0.75	0.24	98,98,98,98	0
3	ACY	A	603	4/4	0.76	0.21	94,94,95,95	0
2	MPD	A	590	8/8	0.76	0.20	50,54,60,62	0
2	MPD	A	592	8/8	0.78	0.17	50,54,60,62	0
3	ACY	A	595	4/4	0.80	0.16	83,83,83,83	0
2	MPD	A	589	8/8	0.83	0.24	50,54,60,62	0
2	MPD	A	602	8/8	0.85	0.20	90,91,91,92	0
2	MPD	A	591	8/8	0.85	0.15	66,69,71,71	0
4	TRS	A	601	8/8	0.85	0.11	74,76,77,77	0
3	ACY	A	596	4/4	0.86	0.16	95,95,95,96	0
3	ACY	A	593	4/4	0.90	0.15	74,74,75,75	0
4	TRS	A	600	8/8	0.92	0.11	68,70,70,71	0

6.5 Other polymers ⓘ

There are no such residues in this entry.