



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:32 AM UTC

PDB ID : 4Z8X / pdb_00004z8x
Title : Truncated FtsH from *A. aeolicus*
Authors : Vostrukhina, M.; Baumann, U.; Schacherl, M.; Bieniossek, C.; Lanz, M.; Baumgartner, R.
Deposited on : 2015-04-09
Resolution : 3.25 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

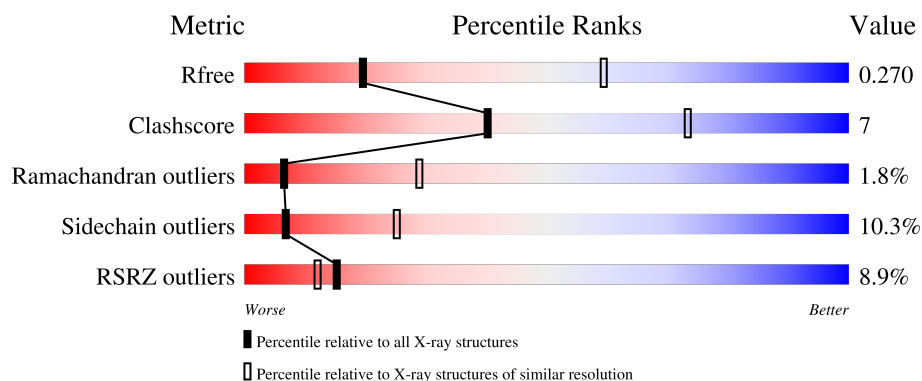
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	497	7% 64% 20% • 14%
1	B	497	8% 62% 21% • 14%
1	C	497	8% 62% 21% • 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10110 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 ATP-dependent zinc metalloprotease FtsH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3351	2137	566	636	12			
1	B	425	Total	C	N	O	S	0	0	0
			3351	2137	566	636	12			
1	C	423	Total	C	N	O	S	0	0	0
			3333	2125	562	634	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLY	-	expression tag	UNP O67077
A	139	SER	-	expression tag	UNP O67077
A	140	HIS	-	expression tag	UNP O67077
A	141	MET	-	expression tag	UNP O67077
A	250	MET	ILE	engineered mutation	UNP O67077
A	360	LEU	PHE	engineered mutation	UNP O67077
A	552	ARG	LYS	engineered mutation	UNP O67077
A	627	GLY	GLU	engineered mutation	UNP O67077
B	138	GLY	-	expression tag	UNP O67077
B	139	SER	-	expression tag	UNP O67077
B	140	HIS	-	expression tag	UNP O67077
B	141	MET	-	expression tag	UNP O67077
B	250	MET	ILE	engineered mutation	UNP O67077
B	360	LEU	PHE	engineered mutation	UNP O67077
B	552	ARG	LYS	engineered mutation	UNP O67077
B	627	GLY	GLU	engineered mutation	UNP O67077
C	138	GLY	-	expression tag	UNP O67077
C	139	SER	-	expression tag	UNP O67077
C	140	HIS	-	expression tag	UNP O67077
C	141	MET	-	expression tag	UNP O67077
C	250	MET	ILE	engineered mutation	UNP O67077
C	360	LEU	PHE	engineered mutation	UNP O67077
C	552	ARG	LYS	engineered mutation	UNP O67077

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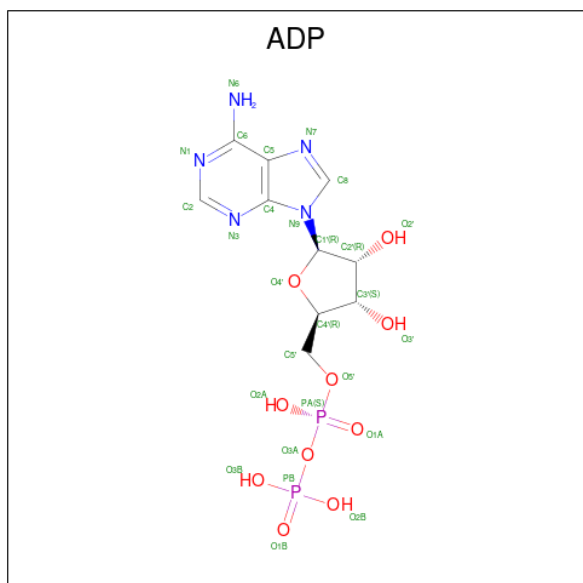
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Chain	Residue	Modelled	Actual	Comment	Reference
C	627	GLY	GLU	engineered mutation	UNP O67077

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

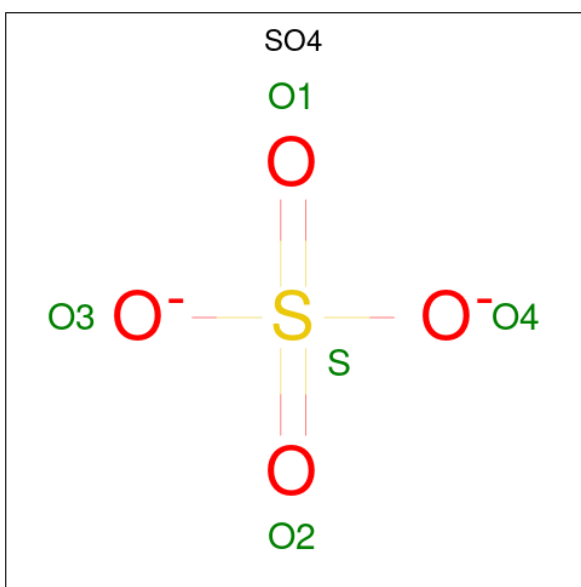
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	27	0
3	C	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

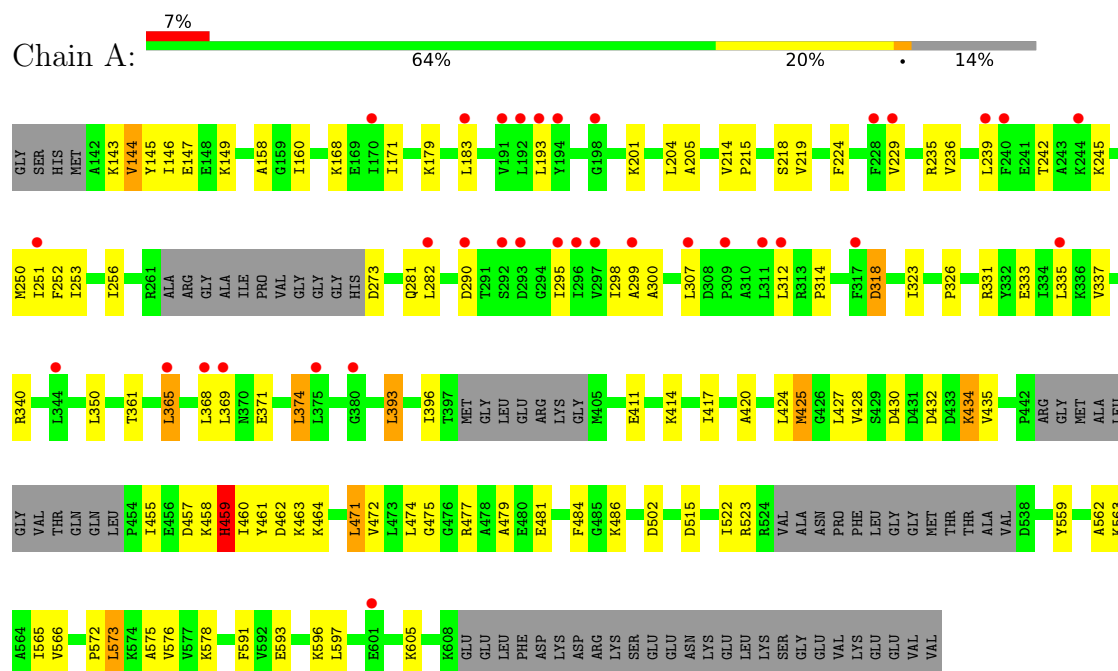
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		

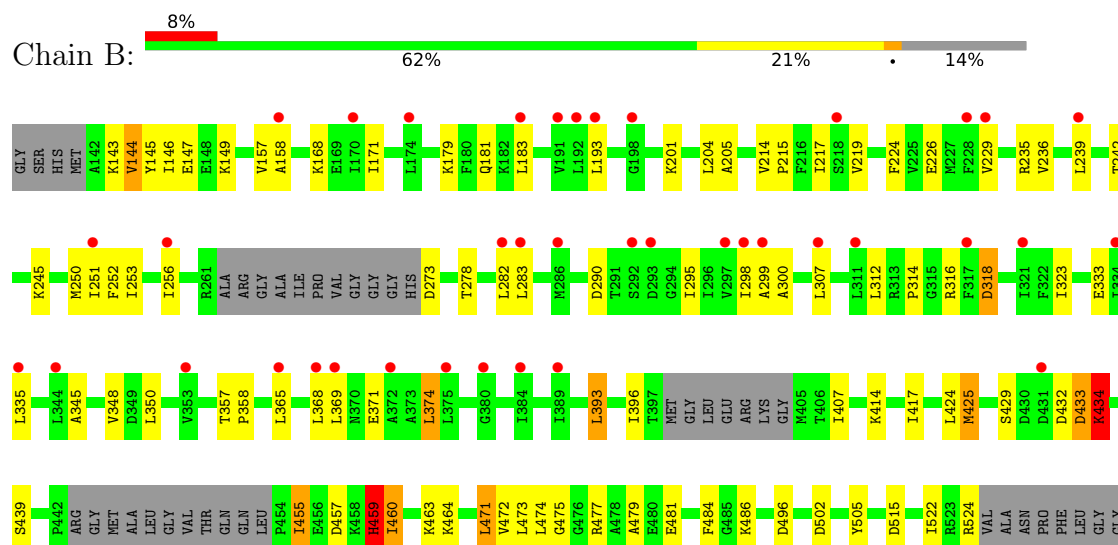
3 Residue-property plots

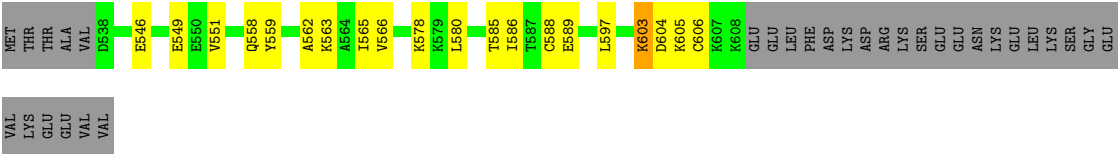
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ATP-dependent zinc metalloprotease FtsH

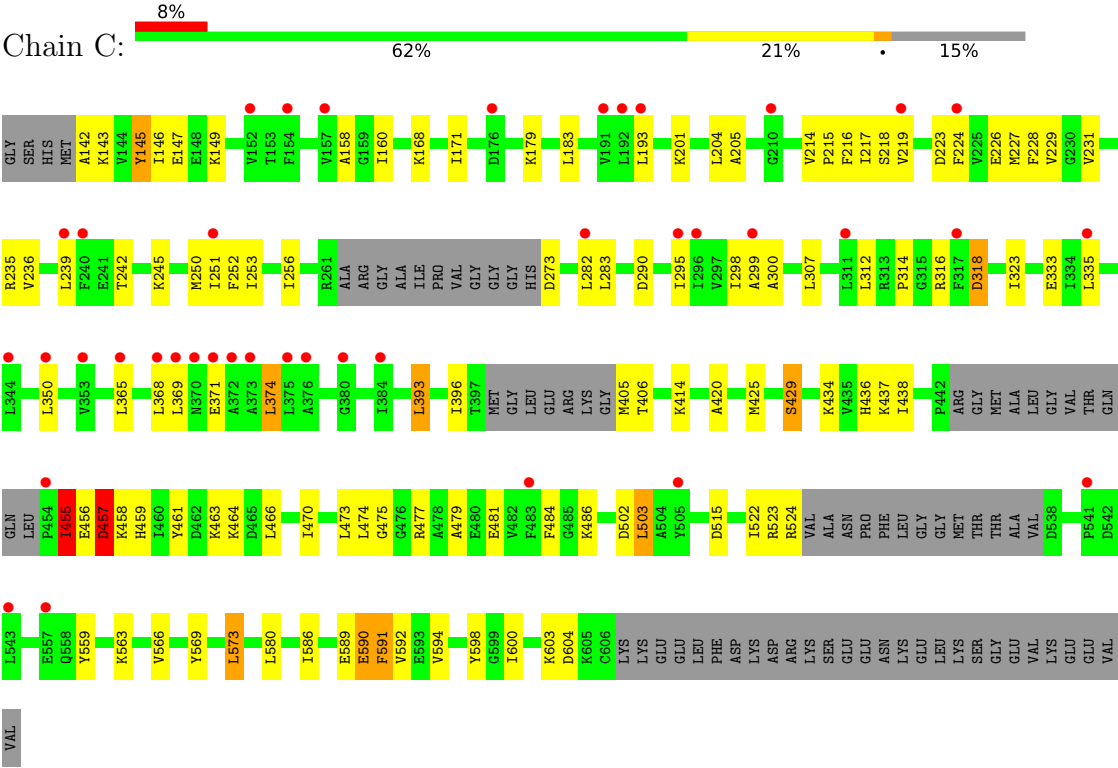


• Molecule 1: ATP-dependent zinc metalloprotease FtsH





● Molecule 1: ATP-dependent zinc metalloprotease FtsH



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	127.86Å 188.48Å 206.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.51 – 3.25 64.51 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (64.51-3.25) 99.3 (64.51-3.25)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.26Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.226 , 0.253 (Not available) , 0.270	Depositor DCC
R_{free} test set	2006 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	124.1	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 215.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10110	wwPDB-VP
Average B, all atoms (Å ²)	221.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.85% 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: ZN, ADP, 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	0.92	0/3399	1.38	14/4568 (0.3%)
1	B	0.91	0/3399	1.36	16/4568 (0.4%)
1	C	0.90	0/3381	1.36	9/4546 (0.2%)
All	All	0.91	0/10179	1.37	39/13682 (0.3%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	HIS	CA-C-N	7.02	134.61	121.97
1	A	459	HIS	C-N-CA	7.02	134.61	121.97
1	B	459	HIS	CA-C-N	7.02	134.60	121.97
1	B	459	HIS	C-N-CA	7.02	134.60	121.97
1	A	434	LYS	CA-C-N	6.81	131.63	123.19
1	A	434	LYS	C-N-CA	6.81	131.63	123.19
1	B	434	LYS	CA-C-N	6.52	131.69	123.14
1	B	434	LYS	C-N-CA	6.52	131.69	123.14
1	B	496	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	462	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	430	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	591	PHE	CA-CB-CG	5.72	119.53	113.80
1	A	235	ARG	CA-C-N	5.64	128.48	120.53
1	A	235	ARG	C-N-CA	5.64	128.48	120.53
1	C	429	SER	CA-C-N	5.62	132.28	121.54
1	C	429	SER	C-N-CA	5.62	132.28	121.54
1	B	235	ARG	CA-C-N	5.61	128.44	120.53
1	B	235	ARG	C-N-CA	5.61	128.44	120.53
1	B	433	ASP	CA-C-N	5.53	132.10	121.54
1	B	433	ASP	C-N-CA	5.53	132.10	121.54
1	A	523	ARG	CA-C-N	5.53	131.65	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	ARG	C-N-CA	5.53	131.65	121.70
1	A	144	VAL	CA-C-N	5.48	132.01	121.54
1	A	144	VAL	C-N-CA	5.48	132.01	121.54
1	A	455	ILE	CA-C-N	5.44	131.94	121.54
1	A	455	ILE	C-N-CA	5.44	131.94	121.54
1	B	429	SER	CA-C-N	5.40	131.85	121.54
1	B	429	SER	C-N-CA	5.40	131.85	121.54
1	C	273	ASP	CA-C-N	5.26	127.85	120.28
1	C	273	ASP	C-N-CA	5.26	127.85	120.28
1	B	589	GLU	CB-CG-CD	5.20	121.44	112.60
1	B	144	VAL	CA-C-N	5.13	131.34	121.54
1	B	144	VAL	C-N-CA	5.13	131.34	121.54
1	B	278	THR	CA-C-N	5.10	127.07	120.44
1	B	278	THR	C-N-CA	5.10	127.07	120.44
1	C	228	PHE	CA-CB-CG	5.09	118.89	113.80
1	C	235	ARG	CA-C-N	5.08	127.69	120.53
1	C	235	ARG	C-N-CA	5.08	127.69	120.53
1	C	457	ASP	CA-CB-CG	5.02	117.62	112.60

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	3351	0	3449	42	0
1	B	3351	0	3449	45	0
1	C	3333	0	3423	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	27	0	12	0	0
3	C	27	0	12	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	10110	0	10345	134	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 (134) 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:B:146:ILE:O	1:B:217:ILE:HA	1.70	0.91
1:B:147:GLU:HG2	1:B:217:ILE:HG12	1.59	0.84
1:C:142:ALA:N	1:C:223:ASP:HB3	2.02	0.76
1:A:424:LEU:HD21	1:A:565:ILE:HG22	1.74	0.69
1:A:479:ALA:HA	1:A:566:VAL:HG11	1.77	0.67
1:A:144:VAL:HB	1:A:219:VAL:HG23	1.82	0.62
1:C:436:HIS:CG	1:C:437:LYS:H	2.17	0.61
1:C:158:ALA:HB1	1:C:333:GLU:HB3	1.81	0.61
1:C:466:LEU:HD22	1:C:503:LEU:HD21	1.83	0.61
1:C:459:HIS:HD2	1:C:461:TYR:CZ	2.18	0.60
1:A:572:PRO:O	1:A:575:ALA:HB3	2.01	0.59
1:B:425:MET:HG3	1:B:471:LEU:HD13	1.84	0.59
1:A:281:GLN:HB2	1:C:227:MET:HE1	1.85	0.58
1:C:205:ALA:HB1	1:C:250:MET:HE1	1.86	0.58
1:A:205:ALA:HB1	1:A:250:MET:HE1	1.87	0.57
1:B:144:VAL:HB	1:B:219:VAL:HG23	1.87	0.57
1:C:335:LEU:HB3	1:C:350:LEU:HD22	1.87	0.57
1:A:427:LEU:HG	1:A:435:VAL:HG21	1.85	0.56
1:B:205:ALA:HB1	1:B:250:MET:HE1	1.87	0.56
1:A:411:GLU:OE2	1:B:459:HIS:HD2	1.88	0.56
1:A:158:ALA:HB1	1:A:333:GLU:HB3	1.87	0.56
1:A:477:ARG:HG3	1:A:559:TYR:CE1	2.42	0.55
1:C:470:ILE:HG13	1:C:503:LEU:HD13	1.89	0.55
1:A:335:LEU:HB3	1:A:350:LEU:HD22	1.89	0.54
1:B:588:CYS:HG	1:B:606:CYS:HG	1.52	0.54
1:B:432:ASP:H	1:B:605:LYS:HZ2	1.54	0.54
1:A:146:ILE:HD13	1:A:218:SER:HB3	1.90	0.53
1:A:420:ALA:HB1	1:A:573:LEU:HD22	1.91	0.53
1:B:603:LYS:HZ2	1:B:604:ASP:H	1.57	0.53
1:B:393:LEU:HA	1:B:396:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ARG:HG3	1:B:559:TYR:CE1	2.45	0.52
1:A:393:LEU:HA	1:A:396:ILE:HD12	1.92	0.51
1:B:149:LYS:HE3	1:B:215:PRO:HG3	1.93	0.51
1:C:477:ARG:HG3	1:C:559:TYR:CE1	2.45	0.51
1:B:580:LEU:HD13	1:B:586:ILE:HG12	1.93	0.51
1:C:393:LEU:HA	1:C:396:ILE:HD12	1.92	0.51
1:B:335:LEU:HB3	1:B:350:LEU:HD22	1.93	0.51
1:C:149:LYS:HE3	1:C:215:PRO:HG3	1.93	0.51
1:A:149:LYS:HE3	1:A:215:PRO:HG3	1.93	0.50
1:C:252:PHE:HA	1:C:298:ILE:O	2.12	0.49
1:B:252:PHE:HA	1:B:298:ILE:O	2.12	0.49
1:C:566:VAL:HG13	1:C:573:LEU:HD12	1.95	0.49
1:A:424:LEU:CD2	1:A:565:ILE:HG22	2.42	0.49
1:A:252:PHE:HA	1:A:298:ILE:O	2.12	0.49
1:C:420:ALA:HB1	1:C:573:LEU:CD2	2.43	0.49
1:C:590:GLU:O	1:C:594:VAL:HG23	2.12	0.48
1:A:559:TYR:CE2	1:A:563:LYS:HD2	2.48	0.48
1:B:158:ALA:HB1	1:B:333:GLU:HB3	1.94	0.48
1:B:559:TYR:CE2	1:B:563:LYS:HD2	2.47	0.48
1:B:459:HIS:O	1:B:460:ILE:HG12	2.14	0.48
1:A:168:LYS:HA	1:A:171:ILE:HD12	1.95	0.47
1:B:588:CYS:SG	1:B:606:CYS:SG	3.07	0.47
1:C:559:TYR:CE2	1:C:563:LYS:HD2	2.49	0.47
1:B:168:LYS:HA	1:B:171:ILE:HD12	1.96	0.47
1:B:242:THR:HA	1:B:245:LYS:HE3	1.95	0.47
1:B:479:ALA:HA	1:B:566:VAL:HG11	1.95	0.47
1:C:168:LYS:HA	1:C:171:ILE:HD12	1.95	0.47
1:C:242:THR:HA	1:C:245:LYS:HE3	1.96	0.47
1:B:471:LEU:HB2	1:B:558:GLN:HE21	1.81	0.47
1:A:242:THR:HA	1:A:245:LYS:HE3	1.96	0.46
1:C:580:LEU:HD13	1:C:586:ILE:HG12	1.97	0.46
1:A:471:LEU:HD22	1:A:562:ALA:HB2	1.99	0.45
1:C:459:HIS:CD2	1:C:461:TYR:CZ	3.03	0.45
1:A:326:PRO:HB2	1:A:331:ARG:HG3	1.98	0.45
1:A:420:ALA:HB1	1:A:573:LEU:CD2	2.46	0.45
1:C:239:LEU:HD21	1:C:251:ILE:HG21	1.98	0.45
1:B:256:ILE:HG21	1:B:299:ALA:HB1	1.99	0.45
1:C:256:ILE:HG21	1:C:299:ALA:HB1	1.99	0.45
1:A:576:VAL:HG11	1:A:591:PHE:CD2	2.52	0.44
1:A:361:THR:O	1:A:365:LEU:HB2	2.18	0.44
1:A:425:MET:HB3	1:A:472:VAL:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LEU:HD21	1:B:251:ILE:HG21	1.98	0.44
1:C:145:TYR:HD1	1:C:219:VAL:HB	1.83	0.44
1:C:146:ILE:HG22	1:C:147:GLU:H	1.81	0.44
1:C:455:ILE:HD11	1:C:473:LEU:HD11	1.99	0.44
1:C:217:ILE:HB	1:C:251:ILE:HA	1.98	0.44
1:C:457:ASP:HB2	1:C:458:LYS:H	1.69	0.44
1:C:436:HIS:CG	1:C:437:LYS:N	2.86	0.44
1:C:479:ALA:HA	1:C:566:VAL:HG11	2.00	0.44
1:A:239:LEU:HD21	1:A:251:ILE:HG21	1.99	0.44
1:A:256:ILE:HG21	1:A:299:ALA:HB1	2.00	0.44
1:B:193:LEU:HD21	1:B:204:LEU:HD23	2.00	0.43
1:B:505:TYR:CE2	1:B:551:VAL:HG11	2.53	0.43
1:A:593:GLU:HA	1:A:596:LYS:HE3	2.01	0.43
1:B:439:SER:HB2	1:B:585:THR:HG23	2.00	0.43
1:B:414:LYS:HD3	1:B:484:PHE:CD2	2.54	0.43
1:A:193:LEU:HD21	1:A:204:LEU:HD23	2.00	0.43
1:C:594:VAL:O	1:C:598:TYR:HD1	2.01	0.43
1:B:236:VAL:HG11	1:B:282:LEU:HA	2.01	0.43
1:C:569:TYR:HD1	1:C:600:ILE:HD13	1.84	0.43
1:A:474:LEU:HD13	1:A:559:TYR:HB2	2.00	0.42
1:C:193:LEU:HD21	1:C:204:LEU:HD23	2.01	0.42
1:C:414:LYS:HD3	1:C:484:PHE:CE2	2.54	0.42
1:C:201:LYS:HD2	1:C:300:ALA:HB1	2.01	0.42
1:C:283:LEU:HB3	1:C:316:ARG:HD3	2.02	0.42
1:B:424:LEU:HD21	1:B:565:ILE:HG22	1.99	0.42
1:C:236:VAL:HG11	1:C:282:LEU:HA	2.00	0.42
1:B:455:ILE:HD13	1:B:455:ILE:N	2.34	0.42
1:A:371:GLU:HA	1:A:374:LEU:HB2	2.02	0.42
1:C:371:GLU:HA	1:C:374:LEU:HB2	2.02	0.42
1:B:546:GLU:O	1:B:549:GLU:HG2	2.20	0.42
1:B:473:LEU:HD23	1:B:473:LEU:HA	1.90	0.42
1:C:405:MET:HB3	1:C:406:THR:H	1.74	0.42
1:C:474:LEU:HD13	1:C:559:TYR:HB2	2.01	0.42
1:A:414:LYS:HD3	1:A:484:PHE:CE2	2.55	0.42
1:B:219:VAL:HG13	1:B:253:ILE:HG23	2.01	0.42
1:B:201:LYS:HD2	1:B:300:ALA:HB1	2.02	0.41
1:A:314:PRO:HA	1:A:318:ASP:HB3	2.01	0.41
1:A:236:VAL:HG11	1:A:282:LEU:HA	2.01	0.41
1:A:201:LYS:HD2	1:A:300:ALA:HB1	2.02	0.41
1:A:414:LYS:HD3	1:A:484:PHE:CD2	2.55	0.41
1:B:425:MET:HB3	1:B:472:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:LYS:HD3	1:C:484:PHE:CD2	2.55	0.41
1:A:219:VAL:HG13	1:A:253:ILE:HG23	2.02	0.41
1:A:459:HIS:HB3	1:A:461:TYR:CE1	2.55	0.41
1:B:371:GLU:HA	1:B:374:LEU:HB2	2.02	0.41
1:B:283:LEU:HD22	1:B:316:ARG:HD3	2.01	0.41
1:B:314:PRO:HA	1:B:318:ASP:HB3	2.02	0.41
1:C:314:PRO:HA	1:C:318:ASP:HB3	2.02	0.41
1:A:337:VAL:HG13	1:A:340:ARG:HH21	1.86	0.41
1:A:427:LEU:HD23	1:A:605:LYS:HB2	2.02	0.41
1:B:358:PRO:HB2	1:B:407:ILE:HB	2.02	0.41
1:B:471:LEU:HD22	1:B:562:ALA:HB2	2.02	0.41
1:C:146:ILE:HD12	1:C:218:SER:HB3	2.03	0.41
1:C:216:PHE:CE2	1:C:218:SER:HB2	2.55	0.41
1:C:420:ALA:HB1	1:C:573:LEU:HD22	2.01	0.41
1:C:219:VAL:HG13	1:C:253:ILE:HG23	2.01	0.41
1:C:438:ILE:HB	1:C:586:ILE:HG13	2.03	0.41
1:B:345:ALA:HB3	1:B:348:VAL:HG13	2.04	0.40
1:B:417:ILE:HD12	1:B:484:PHE:CZ	2.56	0.40
1:A:417:ILE:HD12	1:A:484:PHE:CZ	2.57	0.40
1:B:474:LEU:HD13	1:B:559:TYR:HB2	2.03	0.40
1:C:146:ILE:HG22	1:C:147:GLU:N	2.36	0.40
1:C:459:HIS:HD2	1:C:461:TYR:CE2	2.39	0.40

There are no symmetry-related clashes.

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	415/497 (84%)	379 (91%)	28 (7%)	8 (2%)	6	28
1	B	415/497 (84%)	378 (91%)	31 (8%)	6 (1%)	9	33
1	C	413/497 (83%)	373 (90%)	32 (8%)	8 (2%)	6	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1243/1491 (83%)	1130 (91%)	91 (7%)	22 (2%)	6	29

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	ILE
1	C	434	LYS
1	C	455	ILE
1	C	604	ASP
1	A	147	GLU
1	A	229	VAL
1	B	229	VAL
1	B	460	ILE
1	C	229	VAL
1	C	589	GLU
1	A	145	TYR
1	A	434	LYS
1	A	459	HIS
1	B	434	LYS
1	C	457	ASP
1	C	523	ARG
1	A	458	LYS
1	B	145	TYR
1	B	459	HIS
1	B	475	GLY
1	A	475	GLY
1	C	475	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	360/415 (87%)	327 (91%)	33 (9%)	8	29
1	B	360/415 (87%)	321 (89%)	39 (11%)	6	23
1	C	358/415 (86%)	319 (89%)	39 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1078/1245 (87%)	967 (90%)	111 (10%)	7 25

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LYS
1	A	160	ILE
1	A	179	LYS
1	A	183	LEU
1	A	214	VAL
1	A	224	PHE
1	A	273	ASP
1	A	290	ASP
1	A	295	ILE
1	A	307	LEU
1	A	312	LEU
1	A	318	ASP
1	A	323	ILE
1	A	365	LEU
1	A	368	LEU
1	A	369	LEU
1	A	374	LEU
1	A	393	LEU
1	A	425	MET
1	A	428	VAL
1	A	432	ASP
1	A	457	ASP
1	A	463	LYS
1	A	464	LYS
1	A	471	LEU
1	A	481	GLU
1	A	486	LYS
1	A	502	ASP
1	A	515	ASP
1	A	522	ILE
1	A	573	LEU
1	A	578	LYS
1	A	597	LEU
1	B	143	LYS
1	B	157	VAL
1	B	179	LYS
1	B	181	GLN

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Mol	Chain	Res	Type
1	B	183	LEU
1	B	214	VAL
1	B	224	PHE
1	B	226	GLU
1	B	273	ASP
1	B	290	ASP
1	B	295	ILE
1	B	307	LEU
1	B	312	LEU
1	B	318	ASP
1	B	323	ILE
1	B	357	THR
1	B	365	LEU
1	B	368	LEU
1	B	369	LEU
1	B	374	LEU
1	B	393	LEU
1	B	425	MET
1	B	433	ASP
1	B	434	LYS
1	B	455	ILE
1	B	457	ASP
1	B	459	HIS
1	B	463	LYS
1	B	464	LYS
1	B	471	LEU
1	B	481	GLU
1	B	486	LYS
1	B	502	ASP
1	B	515	ASP
1	B	522	ILE
1	B	524	ARG
1	B	578	LYS
1	B	597	LEU
1	B	603	LYS
1	C	143	LYS
1	C	145	TYR
1	C	160	ILE
1	C	179	LYS
1	C	183	LEU
1	C	214	VAL
1	C	224	PHE

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Mol	Chain	Res	Type
1	C	226	GLU
1	C	231	VAL
1	C	290	ASP
1	C	295	ILE
1	C	307	LEU
1	C	312	LEU
1	C	318	ASP
1	C	323	ILE
1	C	365	LEU
1	C	368	LEU
1	C	369	LEU
1	C	374	LEU
1	C	393	LEU
1	C	425	MET
1	C	429	SER
1	C	455	ILE
1	C	456	GLU
1	C	457	ASP
1	C	463	LYS
1	C	464	LYS
1	C	481	GLU
1	C	486	LYS
1	C	502	ASP
1	C	503	LEU
1	C	515	ASP
1	C	522	ILE
1	C	524	ARG
1	C	573	LEU
1	C	590	GLU
1	C	591	PHE
1	C	592	VAL
1	C	603	LYS

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	281	GLN
1	A	367	ASN
1	A	468	ASN
1	B	277	GLN
1	B	281	GLN
1	B	367	ASN

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Mol	Chain	Res	Type
1	B	370	ASN
1	B	558	GLN
1	C	213	HIS
1	C	281	GLN
1	C	367	ASN
1	C	459	HIS

5.3.3 RNA [i](#)

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](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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	SO4	B	702	-	4,4,4	0.24	0	6,6,6	0.19	0
3	ADP	C	702	-	28,29,29	0.46	0	43,45,45	0.58	0
4	SO4	C	703	-	4,4,4	0.26	0	6,6,6	0.13	0
3	ADP	A	702	-	28,29,29	0.44	0	43,45,45	0.58	0
4	SO4	A	703	-	4,4,4	0.30	0	6,6,6	0.09	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
3	ADP	A	702	-	-	6/16/32/32	0/3/3/3
3	ADP	C	702	-	-	6/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

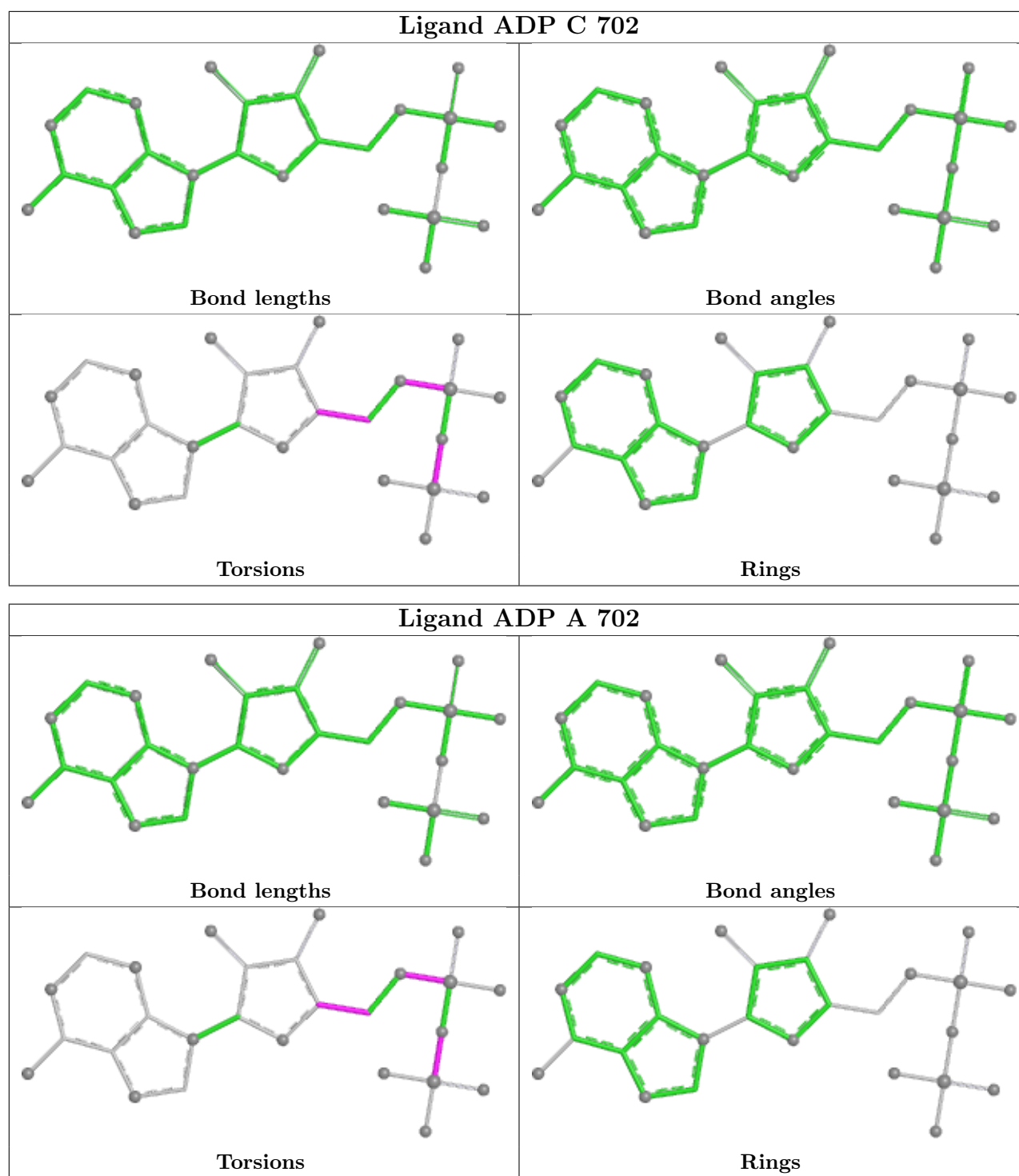
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	ADP	PA-O3A-PB-O3B
3	A	702	ADP	C5'-O5'-PA-O1A
3	A	702	ADP	C5'-O5'-PA-O2A
3	A	702	ADP	C5'-O5'-PA-O3A
3	C	702	ADP	PA-O3A-PB-O3B
3	C	702	ADP	C5'-O5'-PA-O1A
3	C	702	ADP	C5'-O5'-PA-O2A
3	C	702	ADP	C5'-O5'-PA-O3A
3	A	702	ADP	O4'-C4'-C5'-O5'
3	C	702	ADP	O4'-C4'-C5'-O5'
3	A	702	ADP	C3'-C4'-C5'-O5'
3	C	702	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	425/497 (85%)	0.51	34 (8%) 18 14	86, 270, 297, 299	0
1	B	425/497 (85%)	0.53	39 (9%) 14 11	85, 266, 296, 299	0
1	C	423/497 (85%)	0.61	40 (9%) 14 11	95, 273, 295, 298	0
All	All	1273/1491 (85%)	0.55	113 (8%) 15 12	85, 270, 296, 299	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	369	LEU	10.6
1	A	192	LEU	8.0
1	C	368	LEU	7.7
1	B	369	LEU	7.5
1	A	369	LEU	7.1
1	B	368	LEU	6.5
1	C	365	LEU	5.3
1	A	193	LEU	5.2
1	B	192	LEU	5.1
1	C	372	ALA	4.8
1	B	365	LEU	4.8
1	C	296	ILE	4.8
1	C	335	LEU	4.8
1	A	296	ILE	4.4
1	B	170	ILE	4.4
1	C	483	PHE	4.3
1	C	239	LEU	4.2
1	B	299	ALA	4.2
1	B	292	SER	4.1
1	B	372	ALA	4.0
1	A	317	PHE	3.9
1	C	192	LEU	3.9
1	B	317	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	299	ALA	3.9
1	B	297	VAL	3.8
1	B	431	ASP	3.8
1	A	368	LEU	3.8
1	A	191	VAL	3.8
1	A	239	LEU	3.7
1	A	344	LEU	3.7
1	B	353	VAL	3.7
1	C	384	ILE	3.7
1	B	193	LEU	3.7
1	C	251	ILE	3.6
1	B	239	LEU	3.6
1	B	191	VAL	3.5
1	C	376	ALA	3.5
1	A	307	LEU	3.5
1	A	365	LEU	3.4
1	C	317	PHE	3.3
1	C	353	VAL	3.3
1	C	295	ILE	3.3
1	B	298	ILE	3.3
1	A	229	VAL	3.3
1	A	295	ILE	3.3
1	B	307	LEU	3.2
1	B	335	LEU	3.2
1	B	282	LEU	3.1
1	A	335	LEU	3.1
1	C	344	LEU	3.0
1	C	224	PHE	3.0
1	A	170	ILE	3.0
1	C	176	ASP	3.0
1	A	251	ILE	2.9
1	A	311	LEU	2.9
1	B	293	ASP	2.9
1	C	193	LEU	2.9
1	A	282	LEU	2.9
1	A	299	ALA	2.8
1	C	505	TYR	2.8
1	A	601	GLU	2.7
1	A	375	LEU	2.7
1	B	344	LEU	2.7
1	C	282	LEU	2.7
1	C	371	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	373	ALA	2.5
1	C	557	GLU	2.5
1	B	375	LEU	2.5
1	B	218	SER	2.4
1	C	240	PHE	2.4
1	C	191	VAL	2.4
1	B	384	ILE	2.4
1	B	174	LEU	2.4
1	C	541	PRO	2.4
1	B	228	PHE	2.4
1	C	152	VAL	2.4
1	C	380	GLY	2.4
1	A	292	SER	2.4
1	B	311	LEU	2.3
1	B	251	ILE	2.3
1	A	297	VAL	2.3
1	C	311	LEU	2.3
1	A	228	PHE	2.3
1	B	229	VAL	2.3
1	A	309	PRO	2.3
1	C	350	LEU	2.3
1	C	375	LEU	2.2
1	C	157	VAL	2.2
1	A	293	ASP	2.2
1	A	198	GLY	2.2
1	B	380	GLY	2.2
1	A	183	LEU	2.2
1	A	290	ASP	2.2
1	C	154	PHE	2.2
1	B	389	ILE	2.2
1	B	183	LEU	2.2
1	C	370	ASN	2.2
1	B	321	ILE	2.1
1	B	283	LEU	2.1
1	A	244	LYS	2.1
1	C	543	LEU	2.1
1	C	210	GLY	2.1
1	B	286	MET	2.1
1	A	240	PHE	2.1
1	A	194	TYR	2.1
1	C	454	PRO	2.1
1	C	219	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	312	LEU	2.0
1	B	256	ILE	2.0
1	B	158	ALA	2.0
1	A	380	GLY	2.0
1	B	198	GLY	2.0
1	B	334	ILE	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](#)

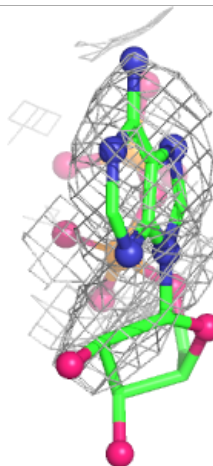
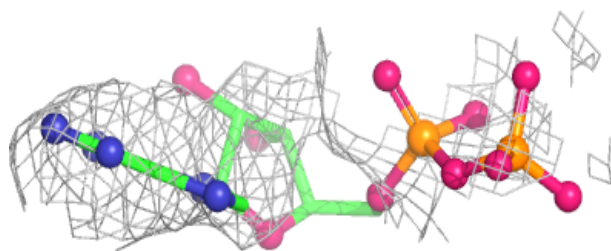
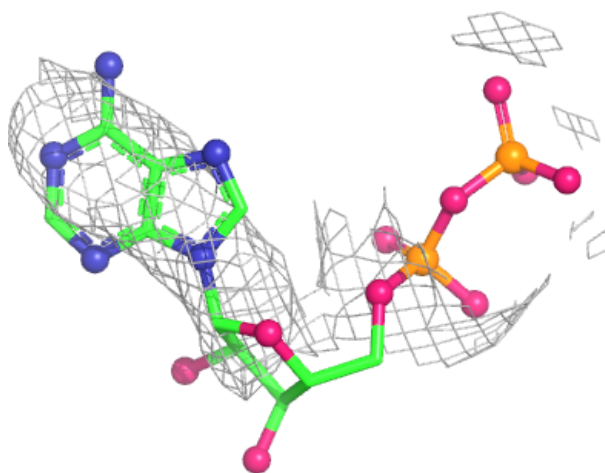
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	C	703	5/5	0.65	0.10	229,229,230,230	0
3	ADP	C	702	27/27	0.70	0.11	299,300,300,300	0
4	SO4	B	702	5/5	0.71	0.10	242,242,242,243	0
3	ADP	A	702	27/27	-	-	139,139,139,139	27
4	SO4	A	703	5/5	0.72	0.09	219,219,220,220	0
2	ZN	B	701	1/1	0.99	0.08	108,108,108,108	0
2	ZN	C	701	1/1	0.99	0.09	126,126,126,126	0
2	ZN	A	701	1/1	0.99	0.04	105,105,105,105	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

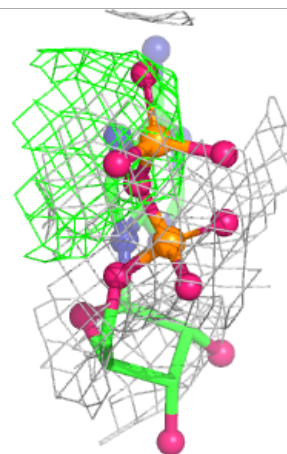
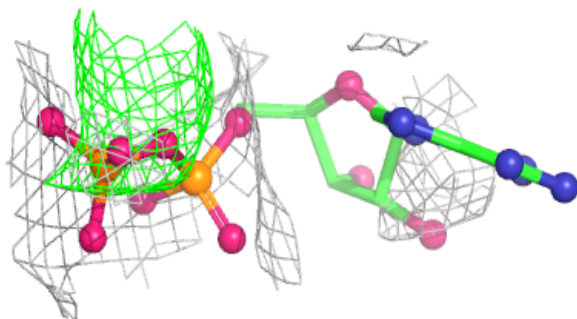
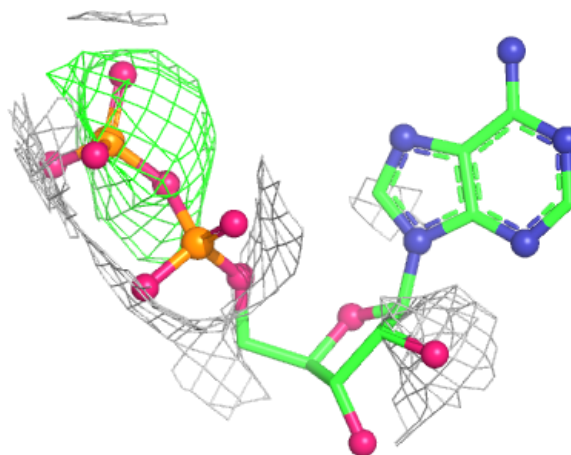
Electron density around ADP C 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.