



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:49 PM GMT

PDB ID : 4Z8X  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

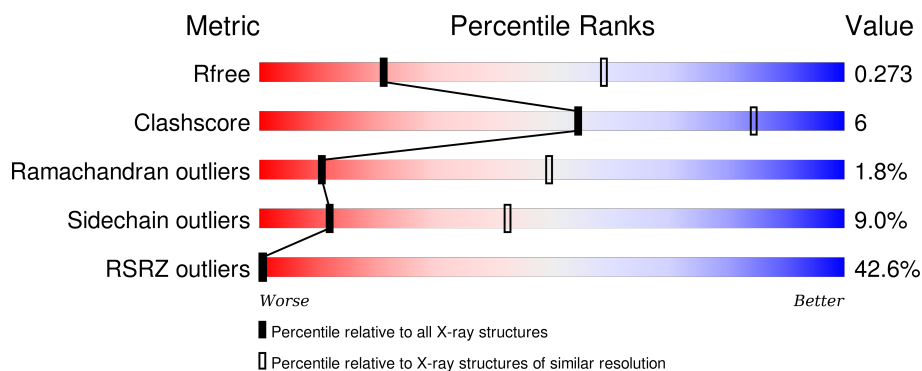
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>38%</div> <div>66%</div> <div>18%</div> <div>•</div> <div>14%</div> </div>
1	B	497	<div> <div>35%</div> <div>65%</div> <div>18%</div> <div>•</div> <div>14%</div> </div>
1	C	497	<div> <div>36%</div> <div>65%</div> <div>19%</div> <div>•</div> <div>15%</div> </div>

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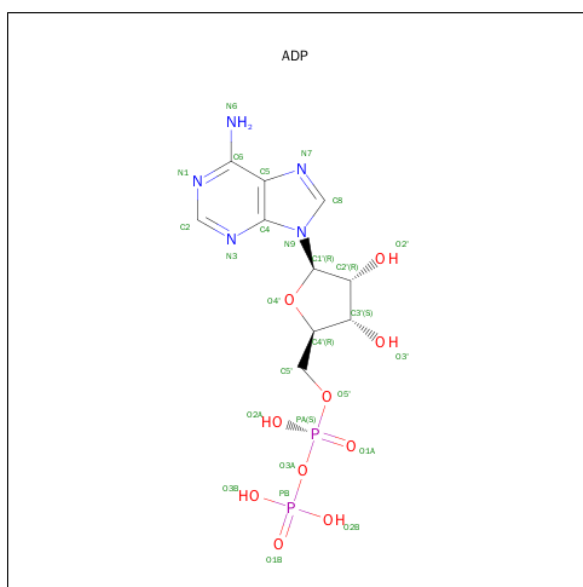
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Chain	Residue	Modelled	Actual	Comment	Reference
C	627	GLY	GLU	engineered mutation	UNP O67077

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

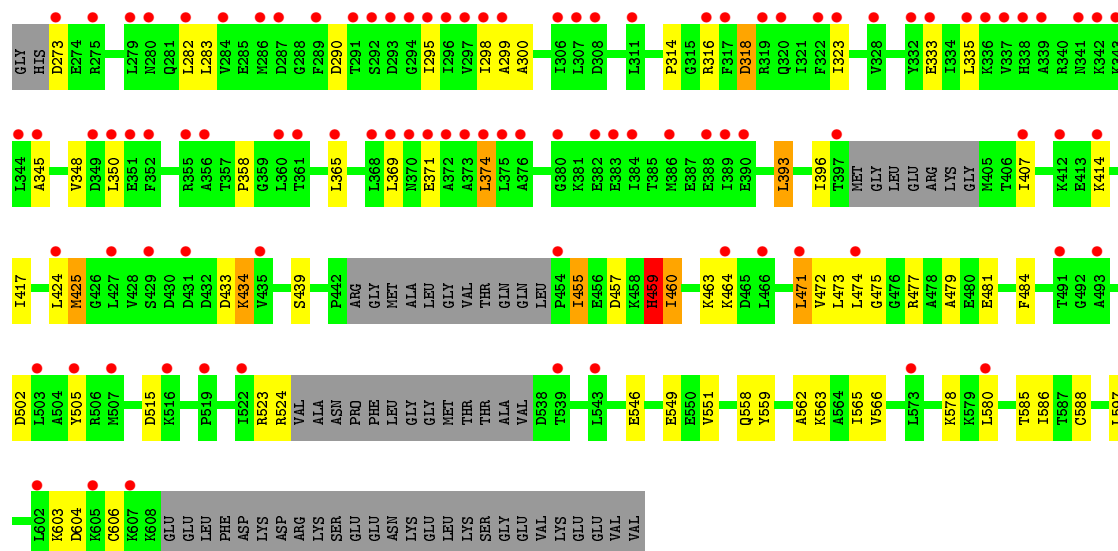


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

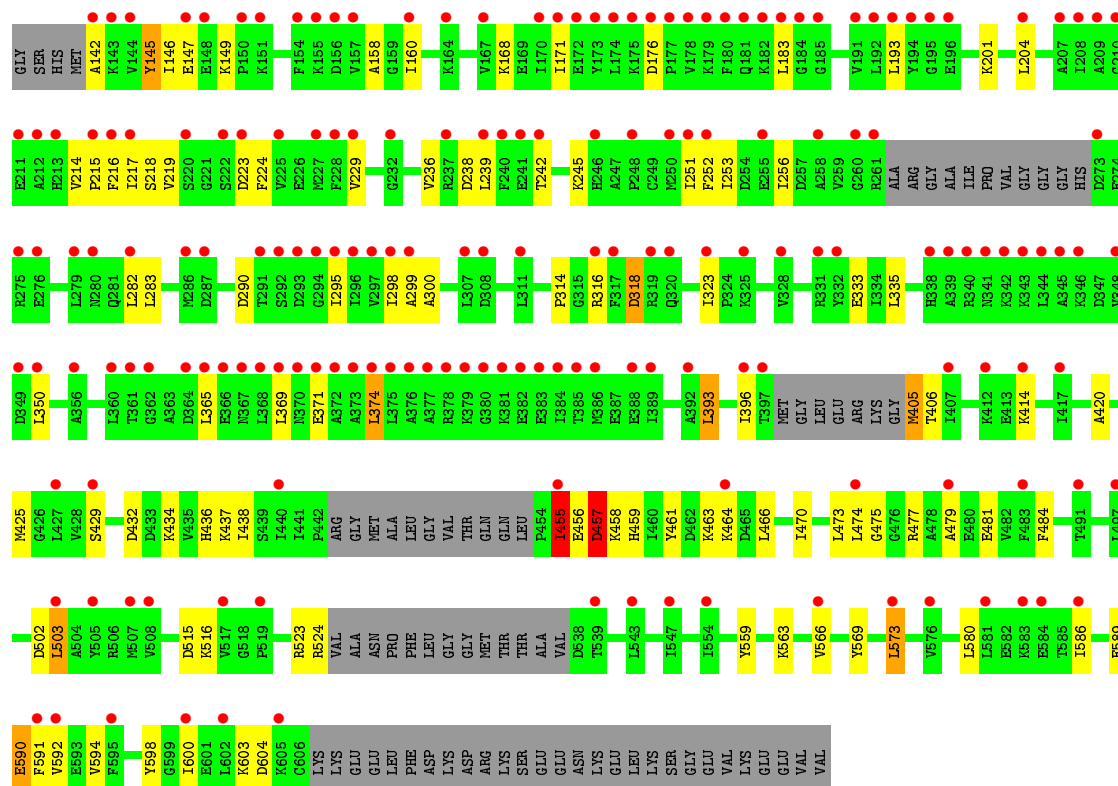
- Molecule 5 is water.

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		





• 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, $\alpha$ , $\beta$ , $\gamma$	127.86 Å   188.48 Å   206.22 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	64.51 – 3.25 94.24 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (64.51-3.25) 99.3 (94.24-3.25)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 3.26 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.226   ,   0.253 0.245   ,   0.273	Depositor DCC
$R_{free}$ test set	2005 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	124.1	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 203.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 39324 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10110	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, ADP

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	0.52	0/3399	0.67	1/4568 (0.0%)
1	B	0.51	0/3399	0.66	1/4568 (0.0%)
1	C	0.50	0/3381	0.66	0/4546
All	All	0.51	0/10179	0.66	2/13682 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	HIS	C-N-CA	5.16	134.61	121.70
1	B	459	HIS	C-N-CA	5.16	134.60	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	41	0
1	B	3351	0	3449	43	0
1	C	3333	0	3423	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	130	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 6.

All (130) 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:466:LEU:HD22	1:C:503:LEU:HD21	1.83	0.61
1:C:158:ALA:HB1	1:C:333:GLU:HB3	1.81	0.61
1:C:459:HIS:HD2	1:C:461:TYR:CZ	2.18	0.60
1:B:425:MET:HG3	1:B:471:LEU:HD13	1.84	0.59
1:A:572:PRO:O	1:A:575:ALA:HB3	2.01	0.59
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: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:C:470:ILE:HG13	1:C:503:LEU:HD13	1.89	0.55
1:A:477:ARG:HG3	1:A:559:TYR:CE1	2.42	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: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:393:LEU:HA	1:B:396:ILE:HD12	1.91	0.52
1:B:477:ARG:HG3	1:B:559:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HA	1:A:396:ILE:HD12	1.92	0.51
1:C:477:ARG:HG3	1:C:559:TYR:CE1	2.45	0.51
1:B:149:LYS:HE3	1:B:215:PRO:HG3	1.93	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:C:149:LYS:HE3	1:C:215:PRO:HG3	1.93	0.51
1:B:335:LEU:HB3	1:B:350:LEU:HD22	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:C:420:ALA:HB1	1:C:573:LEU:CD2	2.43	0.49
1:A:252:PHE:HA	1:A:298:ILE:O	2.12	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: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:A:168:LYS:HA	1:A:171:ILE:HD12	1.95	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:242:THR:HA	1:C:245:LYS:HE3	1.96	0.47
1:C:168:LYS:HA	1:C:171:ILE:HD12	1.95	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:420:ALA:HB1	1:A:573:LEU:CD2	2.46	0.45
1:A:326:PRO:HB2	1:A:331:ARG:HG3	1.98	0.45
1:C:239:LEU:HD21	1:C:251:ILE:HG21	1.98	0.45
1:C:256:ILE:HG21	1:C:299:ALA:HB1	1.99	0.45
1:B:256:ILE:HG21	1:B:299:ALA:HB1	1.99	0.45
1:A:432:ASP:HB2	1:A:605:LYS:HZ3	1.81	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:146:ILE:HG22	1:C:147:GLU:H	1.81	0.44
1:C:145:TYR:HD1	1:C:219:VAL:HB	1.83	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:B:439:SER:HB2	1:B:585:THR:HG23	2.00	0.43
1:A:593:GLU:HA	1:A:596:LYS:HE3	2.01	0.43
1:B:414:LYS:HD3	1:B:484:PHE:CD2	2.54	0.43
1:C:594:VAL:O	1:C:598:TYR:HD1	2.01	0.43
1:A:193:LEU:HD21	1:A:204:LEU:HD23	2.00	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:C:236:VAL:HG11	1:C:282:LEU:HA	2.00	0.42
1:B:424:LEU:HD21	1:B:565:ILE:HG22	1.99	0.42
1:B:455:ILE:N	1:B:455:ILE:HD13	2.34	0.42
1:C:371:GLU:HA	1:C:374:LEU:HB2	2.02	0.42
1:A:371:GLU:HA	1:A:374:LEU:HB2	2.02	0.42
1:B:546:GLU:O	1:B:549:GLU:HG2	2.20	0.42
1:C:474:LEU:HD13	1:C:559:TYR:HB2	2.01	0.42
1:C:405:MET:HB3	1:C:406:THR:H	1.74	0.42
1:B:603:LYS:HZ2	1:B:604:ASP:H	1.67	0.42
1:B:473:LEU:HA	1:B:473:LEU:HD23	1.90	0.42
1:B:219:VAL:HG13	1:B:253:ILE:HG23	2.01	0.42
1:A:414:LYS:HD3	1:A:484:PHE:CE2	2.55	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:414:LYS:HD3	1:A:484:PHE:CD2	2.55	0.41
1:A:201:LYS:HD2	1:A:300:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:MET:HB3	1:B:472:VAL:HA	2.02	0.41
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: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:B:283:LEU:HD22	1:B:316:ARG:HD3	2.01	0.41
1:B:471:LEU:HD22	1:B:562:ALA:HB2	2.02	0.41
1:A:427:LEU:HD23	1:A:605:LYS:HB2	2.02	0.41
1:C:420:ALA:HB1	1:C:573:LEU:HD22	2.01	0.41
1:C:216:PHE:CE2	1:C:218:SER:HB2	2.55	0.41
1:C:146:ILE:HD12	1:C:218:SER:HB3	2.03	0.41
1:B:358:PRO:HB2	1:B:407:ILE:HB	2.02	0.41
1:A:337:VAL:HG13	1:A:340:ARG:HH21	1.86	0.41
1:C:438:ILE:HB	1:C:586:ILE:HG13	2.03	0.41
1:C:219:VAL:HG13	1:C:253:ILE:HG23	2.01	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:C:459:HIS:HD2	1:C:461:TYR:CE2	2.39	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

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%)	10 48
1	B	415/497 (84%)	378 (91%)	31 (8%)	6 (1%)	14 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	413/497 (83%)	373 (90%)	32 (8%)	8 (2%)	10	48
All	All	1243/1491 (83%)	1130 (91%)	91 (7%)	22 (2%)	11	49

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%)	330 (92%)	30 (8%)	14	48
1	B	360/415 (87%)	328 (91%)	32 (9%)	12	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	358/415 (86%)	323 (90%)	35 (10%)	10	38
All	All	1078/1245 (87%)	981 (91%)	97 (9%)	12	42

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ILE
1	A	176	ASP
1	A	183	LEU
1	A	214	VAL
1	A	224	PHE
1	A	273	ASP
1	A	274	GLU
1	A	290	ASP
1	A	295	ILE
1	A	318	ASP
1	A	323	ILE
1	A	365	LEU
1	A	369	LEU
1	A	374	LEU
1	A	393	LEU
1	A	425	MET
1	A	430	ASP
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	502	ASP
1	A	515	ASP
1	A	516	LYS
1	A	522	ILE
1	A	573	LEU
1	A	578	LYS
1	A	597	LEU
1	B	143	LYS
1	B	176	ASP
1	B	181	GLN
1	B	183	LEU
1	B	214	VAL
1	B	224	PHE

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Mol	Chain	Res	Type
1	B	226	GLU
1	B	273	ASP
1	B	290	ASP
1	B	295	ILE
1	B	318	ASP
1	B	323	ILE
1	B	365	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	502	ASP
1	B	515	ASP
1	B	523	ARG
1	B	524	ARG
1	B	578	LYS
1	B	597	LEU
1	C	145	TYR
1	C	160	ILE
1	C	176	ASP
1	C	183	LEU
1	C	214	VAL
1	C	224	PHE
1	C	238	ASP
1	C	290	ASP
1	C	295	ILE
1	C	318	ASP
1	C	323	ILE
1	C	365	LEU
1	C	369	LEU
1	C	374	LEU
1	C	393	LEU
1	C	405	MET

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Mol	Chain	Res	Type
1	C	425	MET
1	C	429	SER
1	C	432	ASP
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	502	ASP
1	C	503	LEU
1	C	515	ASP
1	C	516	LYS
1	C	524	ARG
1	C	573	LEU
1	C	590	GLU
1	C	591	PHE
1	C	592	VAL
1	C	603	LYS

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

Mol	Chain	Res	Type
1	A	468	ASN
1	B	370	ASN
1	B	468	ASN
1	B	558	GLN
1	C	459	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

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	$\# Z  > 2$
3	ADP	A	702	-	22,29,29	0.68	0	27,45,45	0.74	0
4	SO4	A	703	-	4,4,4	0.18	0	6,6,6	0.09	0
4	SO4	B	702	-	4,4,4	0.17	0	6,6,6	0.13	0
3	ADP	C	702	-	22,29,29	0.67	0	27,45,45	0.73	0
4	SO4	C	703	-	4,4,4	0.10	0	6,6,6	0.17	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	-	-	0/12/32/32	0/3/3/3
4	SO4	A	703	-	-	0/0/0/0	0/0/0/0
4	SO4	B	702	-	-	0/0/0/0	0/0/0/0
3	ADP	C	702	-	-	0/12/32/32	0/3/3/3
4	SO4	C	703	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	425/497 (85%)	3.01	191 (44%) 0 0	86, 270, 297, 299	0
1	B	425/497 (85%)	2.62	172 (40%) 0 1	85, 266, 296, 299	0
1	C	423/497 (85%)	2.92	179 (42%) 0 0	95, 273, 295, 298	0
All	All	1273/1491 (85%)	2.85	542 (42%) 0 0	85, 270, 296, 299	0

All (542) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	371	GLU	25.6
1	C	296	ILE	25.3
1	A	296	ILE	23.3
1	C	182	LYS	21.9
1	A	230	GLY	20.8
1	A	369	LEU	20.8
1	A	344	LEU	19.9
1	B	226	GLU	19.3
1	A	229	VAL	18.5
1	A	193	LEU	16.5
1	A	228	PHE	16.2
1	A	185	GLY	16.2
1	A	192	LEU	15.6
1	C	368	LEU	15.6
1	C	382	GLU	15.0
1	C	370	ASN	14.8
1	A	295	ILE	14.3
1	B	344	LEU	14.1
1	A	191	VAL	13.7
1	C	183	LEU	13.6
1	B	369	LEU	13.5
1	B	293	ASP	13.5
1	A	294	GLY	13.4

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Mol	Chain	Res	Type	RSRZ
1	A	184	GLY	13.4
1	C	195	GLY	13.2
1	B	292	SER	13.1
1	B	297	VAL	13.0
1	B	368	LEU	12.9
1	B	191	VAL	12.9
1	B	372	ALA	12.9
1	C	228	PHE	12.6
1	A	227	MET	12.4
1	C	143	LYS	12.1
1	C	372	ALA	12.1
1	C	157	VAL	12.0
1	A	250	MET	12.0
1	B	227	MET	11.8
1	C	250	MET	11.8
1	B	144	VAL	11.7
1	C	208	ILE	11.5
1	C	184	GLY	11.5
1	C	375	LEU	11.3
1	B	365	LEU	11.3
1	A	343	LYS	11.2
1	A	248	PRO	11.2
1	B	192	LEU	11.1
1	A	226	GLU	11.1
1	B	193	LEU	11.0
1	C	191	VAL	11.0
1	C	376	ALA	10.9
1	A	208	ILE	10.9
1	B	208	ILE	10.8
1	C	212	ALA	10.8
1	A	372	ALA	10.8
1	C	343	LYS	10.8
1	C	180	PHE	10.7
1	C	273	ASP	10.7
1	A	376	ALA	10.6
1	B	228	PHE	10.5
1	B	370	ASN	10.3
1	A	180	PHE	10.3
1	B	157	VAL	10.3
1	B	194	TYR	10.2
1	A	292	SER	10.1
1	A	380	GLY	10.1

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Mol	Chain	Res	Type	RSRZ
1	A	297	VAL	10.1
1	A	317	PHE	10.0
1	B	383	GLU	10.0
1	C	380	GLY	10.0
1	A	368	LEU	9.8
1	C	365	LEU	9.6
1	A	247	ALA	9.6
1	C	261	ARG	9.6
1	B	296	ILE	9.5
1	C	297	VAL	9.4
1	B	170	ILE	9.4
1	B	222	SER	9.4
1	B	185	GLY	9.3
1	C	374	LEU	9.3
1	A	342	LYS	9.2
1	C	175	LYS	9.2
1	A	307	LEU	9.1
1	A	167	VAL	9.0
1	C	185	GLY	9.0
1	C	369	LEU	9.0
1	C	383	GLU	8.9
1	A	183	LEU	8.9
1	C	179	LYS	8.9
1	B	151	LYS	8.8
1	C	210	GLY	8.8
1	C	339	ALA	8.8
1	A	365	LEU	8.7
1	C	232	GLY	8.6
1	B	295	ILE	8.6
1	A	231	VAL	8.6
1	A	147	GLU	8.4
1	A	171	ILE	8.4
1	B	180	PHE	8.4
1	B	147	GLU	8.4
1	A	157	VAL	8.4
1	C	295	ILE	8.4
1	B	176	ASP	8.2
1	A	332	TYR	8.2
1	C	239	LEU	8.2
1	C	193	LEU	8.2
1	A	194	TYR	8.2
1	C	240	PHE	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	375	LEU	8.1
1	A	220	SER	8.1
1	C	229	VAL	8.1
1	A	179	LYS	8.0
1	C	328	VAL	7.9
1	C	241	GLU	7.9
1	C	294	GLY	7.9
1	B	182	LYS	7.8
1	A	389	ILE	7.8
1	A	212	ALA	7.8
1	C	344	LEU	7.8
1	A	195	GLY	7.8
1	C	292	SER	7.8
1	B	286	MET	7.7
1	A	170	ILE	7.7
1	B	261	ARG	7.6
1	B	145	TYR	7.6
1	A	383	GLU	7.6
1	C	373	ALA	7.5
1	C	211	GLU	7.5
1	A	215	PRO	7.5
1	A	370	ASN	7.4
1	A	239	LEU	7.4
1	C	384	ILE	7.4
1	C	317	PHE	7.3
1	B	294	GLY	7.3
1	C	192	LEU	7.3
1	A	175	LYS	7.2
1	A	246	HIS	7.2
1	C	215	PRO	7.1
1	B	351	GLU	7.0
1	B	291	THR	7.0
1	C	377	ALA	7.0
1	C	147	GLU	6.9
1	A	345	ALA	6.9
1	B	343	LYS	6.9
1	C	176	ASP	6.8
1	C	155	LYS	6.8
1	C	396	ILE	6.8
1	C	150	PRO	6.7
1	B	317	PHE	6.7
1	B	350	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	163	VAL	6.7
1	B	154	PHE	6.7
1	A	174	LEU	6.6
1	B	375	LEU	6.6
1	A	252	PHE	6.6
1	B	183	LEU	6.5
1	B	273	ASP	6.4
1	C	602	LEU	6.4
1	C	348	VAL	6.4
1	C	170	ILE	6.4
1	B	237	ARG	6.4
1	C	142	ALA	6.3
1	B	240	PHE	6.3
1	C	227	MET	6.3
1	B	239	LEU	6.2
1	C	148	GLU	6.2
1	C	174	LEU	6.2
1	A	384	ILE	6.2
1	B	241	GLU	6.2
1	A	173	TYR	6.1
1	C	286	MET	6.1
1	B	167	VAL	6.1
1	B	179	LYS	6.1
1	B	376	ALA	6.0
1	A	306	ILE	6.0
1	B	336	LYS	6.0
1	A	143	LYS	6.0
1	A	361	THR	6.0
1	B	173	TYR	5.9
1	B	216	PHE	5.9
1	A	144	VAL	5.9
1	B	299	ALA	5.9
1	C	299	ALA	5.9
1	A	176	ASP	5.9
1	C	154	PHE	5.9
1	B	225	VAL	5.8
1	A	293	ASP	5.8
1	B	243	ALA	5.8
1	C	251	ILE	5.8
1	C	222	SER	5.7
1	A	311	LEU	5.7
1	A	150	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	275	ARG	5.6
1	A	182	LYS	5.6
1	C	275	ARG	5.6
1	C	338	HIS	5.6
1	A	280	ASN	5.6
1	C	181	GLN	5.6
1	B	171	ILE	5.5
1	A	273	ASP	5.5
1	A	241	GLU	5.5
1	C	167	VAL	5.5
1	A	381	LYS	5.4
1	A	142	ALA	5.4
1	B	388	GLU	5.4
1	A	232	GLY	5.4
1	A	238	ASP	5.3
1	C	293	ASP	5.3
1	B	275	ARG	5.3
1	B	607	LYS	5.3
1	A	289	PHE	5.2
1	B	352	PHE	5.2
1	C	291	THR	5.2
1	A	349	ASP	5.2
1	C	307	LEU	5.2
1	B	143	LYS	5.2
1	A	163	VAL	5.1
1	A	211	GLU	5.0
1	A	199	VAL	5.0
1	C	237	ARG	5.0
1	C	385	THR	5.0
1	B	389	ILE	5.0
1	B	373	ALA	5.0
1	B	386	MET	4.9
1	B	319	ARG	4.9
1	B	169	GLU	4.9
1	A	350	LEU	4.9
1	B	229	VAL	4.9
1	A	298	ILE	4.8
1	C	156	ASP	4.8
1	A	245	LYS	4.8
1	A	249	CYS	4.8
1	A	251	ILE	4.8
1	B	298	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	379	LYS	4.7
1	C	216	PHE	4.7
1	B	244	LYS	4.7
1	B	339	ALA	4.7
1	A	196	GLU	4.6
1	C	298	ILE	4.6
1	B	307	LEU	4.6
1	B	236	VAL	4.6
1	C	252	PHE	4.6
1	B	320	GLN	4.6
1	B	335	LEU	4.6
1	C	248	PRO	4.6
1	B	337	VAL	4.6
1	A	217	ILE	4.6
1	B	308	ASP	4.5
1	C	350	LEU	4.5
1	C	361	THR	4.5
1	A	286	MET	4.5
1	B	342	LYS	4.4
1	C	279	LEU	4.4
1	A	237	ARG	4.4
1	B	328	VAL	4.4
1	B	384	ILE	4.4
1	A	209	ALA	4.3
1	A	308	ASP	4.3
1	B	306	ILE	4.3
1	C	213	HIS	4.3
1	A	154	PHE	4.3
1	C	346	LYS	4.3
1	A	216	PHE	4.3
1	A	388	GLU	4.3
1	B	250	MET	4.3
1	A	189	LYS	4.3
1	C	276	GLU	4.3
1	C	173	TYR	4.3
1	A	360	LEU	4.3
1	A	377	ALA	4.2
1	B	175	LYS	4.2
1	C	308	ASP	4.2
1	A	152	VAL	4.2
1	C	223	ASP	4.1
1	B	247	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	156	ASP	4.1
1	B	211	GLU	4.1
1	A	223	ASP	4.1
1	C	364	ASP	4.1
1	C	381	LYS	4.1
1	A	240	PHE	4.1
1	A	214	VAL	4.1
1	A	315	GLY	4.0
1	B	382	GLU	4.0
1	C	209	ALA	4.0
1	C	389	ILE	4.0
1	C	280	ASN	4.0
1	C	591	PHE	4.0
1	C	367	ASN	4.0
1	B	204	LEU	3.9
1	C	204	LEU	3.9
1	C	217	ILE	3.9
1	A	319	ARG	3.9
1	C	412	LYS	3.9
1	A	158	ALA	3.8
1	C	388	GLU	3.8
1	A	328	VAL	3.8
1	B	152	VAL	3.8
1	A	385	THR	3.7
1	A	393	LEU	3.7
1	A	323	ILE	3.7
1	C	417	ILE	3.7
1	A	304	PRO	3.7
1	A	225	VAL	3.6
1	C	194	TYR	3.6
1	B	249	CYS	3.6
1	B	341	ASN	3.6
1	A	181	GLN	3.6
1	C	342	LYS	3.6
1	C	258	ALA	3.5
1	B	602	LEU	3.5
1	A	172	GLU	3.5
1	A	224	PHE	3.5
1	A	145	TYR	3.5
1	A	186	ARG	3.5
1	B	349	ASP	3.5
1	A	291	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	319	ARG	3.5
1	B	246	HIS	3.4
1	B	431	ASP	3.4
1	A	382	GLU	3.4
1	A	390	GLU	3.4
1	C	151	LYS	3.4
1	B	371	GLU	3.4
1	C	474	LEU	3.4
1	B	280	ASN	3.4
1	B	199	VAL	3.4
1	C	583	LYS	3.4
1	C	507	MET	3.3
1	C	427	LEU	3.3
1	C	505	TYR	3.3
1	C	332	TYR	3.3
1	A	206	LYS	3.3
1	B	361	THR	3.3
1	B	289	PHE	3.3
1	A	396	ILE	3.3
1	C	331	ARG	3.3
1	A	204	LEU	3.3
1	A	407	ILE	3.2
1	A	221	GLY	3.2
1	A	379	LYS	3.2
1	B	397	THR	3.2
1	B	287	ASP	3.2
1	C	386	MET	3.2
1	B	258	ALA	3.2
1	C	345	ALA	3.2
1	C	196	GLU	3.1
1	B	217	ILE	3.1
1	B	284	VAL	3.1
1	B	150	PRO	3.1
1	C	483	PHE	3.1
1	B	435	VAL	3.1
1	A	213	HIS	3.1
1	C	366	GLU	3.1
1	A	543	LEU	3.1
1	B	252	PHE	3.1
1	B	190	GLY	3.1
1	A	346	LYS	3.1
1	C	177	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	189	LYS	3.0
1	C	260	GLY	3.0
1	B	539	THR	3.0
1	C	242	THR	3.0
1	B	230	GLY	3.0
1	C	349	ASP	3.0
1	B	209	ALA	3.0
1	C	360	LEU	3.0
1	B	332	TYR	3.0
1	C	246	HIS	3.0
1	A	312	LEU	3.0
1	B	184	GLY	3.0
1	B	196	GLU	3.0
1	C	455	ILE	3.0
1	A	156	ASP	2.9
1	A	282	LEU	2.9
1	B	374	LEU	2.9
1	C	566	VAL	2.9
1	C	397	THR	2.9
1	C	311	LEU	2.9
1	B	153	THR	2.9
1	B	407	ILE	2.9
1	B	215	PRO	2.9
1	C	316	ARG	2.9
1	A	438	ILE	2.8
1	A	335	LEU	2.8
1	A	299	ALA	2.8
1	B	311	LEU	2.8
1	B	466	LEU	2.8
1	C	519	PRO	2.8
1	A	522	ILE	2.8
1	B	543	LEU	2.8
1	A	222	SER	2.7
1	C	543	LEU	2.7
1	A	573	LEU	2.7
1	A	440	ILE	2.7
1	B	390	GLU	2.7
1	A	338	HIS	2.7
1	C	595	PHE	2.7
1	B	218	SER	2.7
1	C	255	GLU	2.7
1	A	580	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	151	LYS	2.7
1	C	440	ILE	2.7
1	A	358	PRO	2.7
1	C	172	GLU	2.7
1	C	378	ARG	2.6
1	A	316	ARG	2.6
1	C	517	VAL	2.6
1	A	539	THR	2.6
1	A	508	VAL	2.6
1	B	146	ILE	2.6
1	C	464	LYS	2.6
1	C	362	GLY	2.6
1	A	454	PRO	2.6
1	C	282	LEU	2.6
1	A	190	GLY	2.6
1	B	323	ILE	2.6
1	A	309	PRO	2.6
1	C	207	ALA	2.6
1	A	210	GLY	2.6
1	A	566	VAL	2.6
1	B	168	LYS	2.5
1	A	547	ILE	2.5
1	B	580	LEU	2.5
1	C	586	ILE	2.5
1	A	441	ILE	2.5
1	B	516	LYS	2.5
1	B	474	LEU	2.5
1	A	177	PRO	2.5
1	B	186	ARG	2.5
1	C	592	VAL	2.5
1	B	174	LEU	2.5
1	A	155	LYS	2.5
1	B	177	PRO	2.4
1	C	340	ARG	2.4
1	A	474	LEU	2.4
1	B	181	GLN	2.4
1	A	456	GLU	2.4
1	B	333	GLU	2.4
1	B	316	ARG	2.4
1	B	505	TYR	2.4
1	B	519	PRO	2.4
1	B	282	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	497	LEU	2.4
1	A	243	ALA	2.4
1	B	212	ALA	2.4
1	A	509	SER	2.4
1	B	454	PRO	2.4
1	A	205	ALA	2.4
1	B	503	LEU	2.4
1	C	144	VAL	2.3
1	A	414	LYS	2.3
1	C	225	VAL	2.3
1	C	341	ASN	2.3
1	B	491	THR	2.3
1	A	188	PRO	2.3
1	A	261	ARG	2.3
1	C	160	ILE	2.3
1	C	576	VAL	2.3
1	C	491	THR	2.3
1	A	330	GLY	2.3
1	A	551	VAL	2.3
1	A	586	ILE	2.3
1	A	160	ILE	2.3
1	B	356	ALA	2.3
1	C	547	ILE	2.3
1	C	539	THR	2.3
1	A	378	ARG	2.3
1	C	323	ILE	2.3
1	B	223	ASP	2.3
1	B	206	LYS	2.3
1	A	524	ARG	2.3
1	C	573	LEU	2.3
1	C	164	LYS	2.3
1	A	146	ILE	2.3
1	C	605	LYS	2.3
1	C	220	SER	2.3
1	A	602	LEU	2.2
1	B	360	LEU	2.2
1	B	471	LEU	2.2
1	C	508	VAL	2.2
1	C	503	LEU	2.2
1	C	554	ILE	2.2
1	B	605	LYS	2.2
1	B	195	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	387	GLU	2.2
1	B	464	LYS	2.2
1	B	322	PHE	2.2
1	A	364	ASP	2.2
1	A	373	ALA	2.2
1	B	355	ARG	2.2
1	C	171	ILE	2.2
1	C	178	VAL	2.2
1	A	148	GLU	2.2
1	C	356	ALA	2.2
1	A	424	LEU	2.2
1	B	279	LEU	2.2
1	B	200	GLY	2.2
1	B	380	GLY	2.2
1	A	520	ILE	2.2
1	C	584	GLU	2.2
1	A	519	PRO	2.1
1	B	414	LYS	2.1
1	C	320	GLN	2.1
1	A	601	GLU	2.1
1	B	412	LYS	2.1
1	B	427	LEU	2.1
1	A	165	GLU	2.1
1	A	546	GLU	2.1
1	A	555	ILE	2.1
1	A	371	GLU	2.1
1	A	491	THR	2.1
1	B	507	MET	2.1
1	B	429	SER	2.1
1	C	429	SER	2.1
1	C	479	ALA	2.1
1	A	538	ASP	2.1
1	C	581	LEU	2.1
1	A	341	ASN	2.1
1	A	600	ILE	2.1
1	B	251	ILE	2.1
1	C	600	ILE	2.1
1	A	427	LEU	2.1
1	B	573	LEU	2.1
1	B	522	ILE	2.0
1	C	407	ILE	2.0
1	B	220	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	497	LEU	2.0
1	C	414	LYS	2.0
1	A	493	ALA	2.0
1	B	338	HIS	2.0
1	C	287	ASP	2.0
1	B	493	ALA	2.0
1	C	392	ALA	2.0
1	B	424	LEU	2.0
1	B	260	GLY	2.0
1	A	287	ASP	2.0
1	C	325	LYS	2.0
1	A	507	MET	2.0
1	B	345	ALA	2.0
1	A	352	PHE	2.0
1	A	595	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ADP	C	702	27/27	0.59	0.29	-0.49	299,300,300,300	0
4	SO4	A	703	5/5	0.82	0.25	-1.14	219,219,220,220	0
4	SO4	B	702	5/5	0.88	0.19	-2.02	242,242,242,243	0
3	ADP	A	702	27/27	-	-	-	139,139,139,139	27
4	SO4	C	703	5/5	0.64	0.20	-	229,229,230,230	0
2	ZN	B	701	1/1	0.93	0.38	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	701	1/1	0.91	0.35	-	105,105,105,105	0
2	ZN	C	701	1/1	0.94	0.39	-	126,126,126,126	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.