



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:27 AM GMT

PDB ID : 1F48
Title : CRYSTAL STRUCTURE OF THE ESCHERICHIA COLI ARSENITE-TRANSLOCATING ATPASE
Authors : Zhou, T.; Radaev, S.; Rosen, B.P.; Gatti, D.L.
Deposited on : 2000-06-07
Resolution : 2.30 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

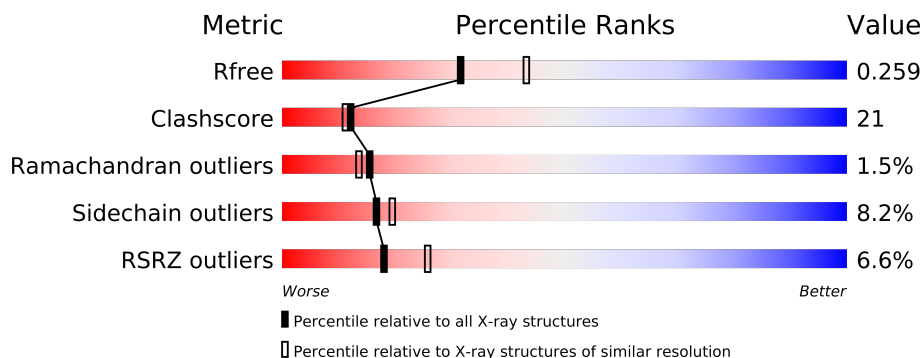
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	589	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	SBO	A	701	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4467 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ARSENITE-TRANSLOCATINGATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4178	2629	737	797	15			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASN	ILE	SEE REMARK 999	UNP P08690
A	584	HIS	-	EXPRESSION TAG	UNP P08690
A	585	HIS	-	EXPRESSION TAG	UNP P08690
A	586	HIS	-	EXPRESSION TAG	UNP P08690
A	587	HIS	-	EXPRESSION TAG	UNP P08690
A	588	HIS	-	EXPRESSION TAG	UNP P08690
A	589	HIS	-	EXPRESSION TAG	UNP P08690

- Molecule 2 is ANTIMONY (III) ION (three-letter code: SB) (formula: Sb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Sb	0	0
			3	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

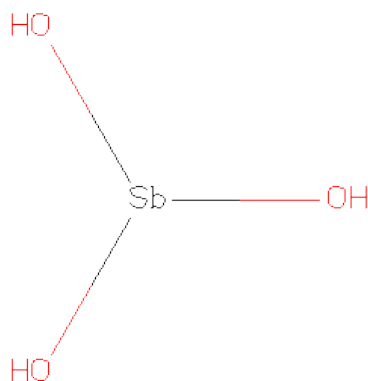
- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	Cd	0	0
			6	6		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

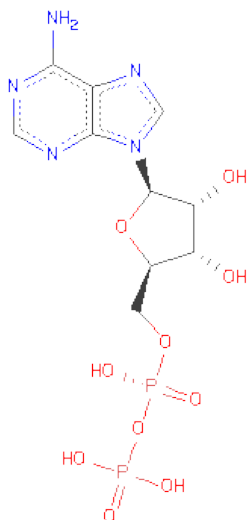
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	3	Total	Cl		0	0
			3	3			

- Molecule 6 is TRIHYDROXYANTIMONITE(III) (three-letter code: SBO) (formula: H₃O₃Sb).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	Sb	0	0
			4	3	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

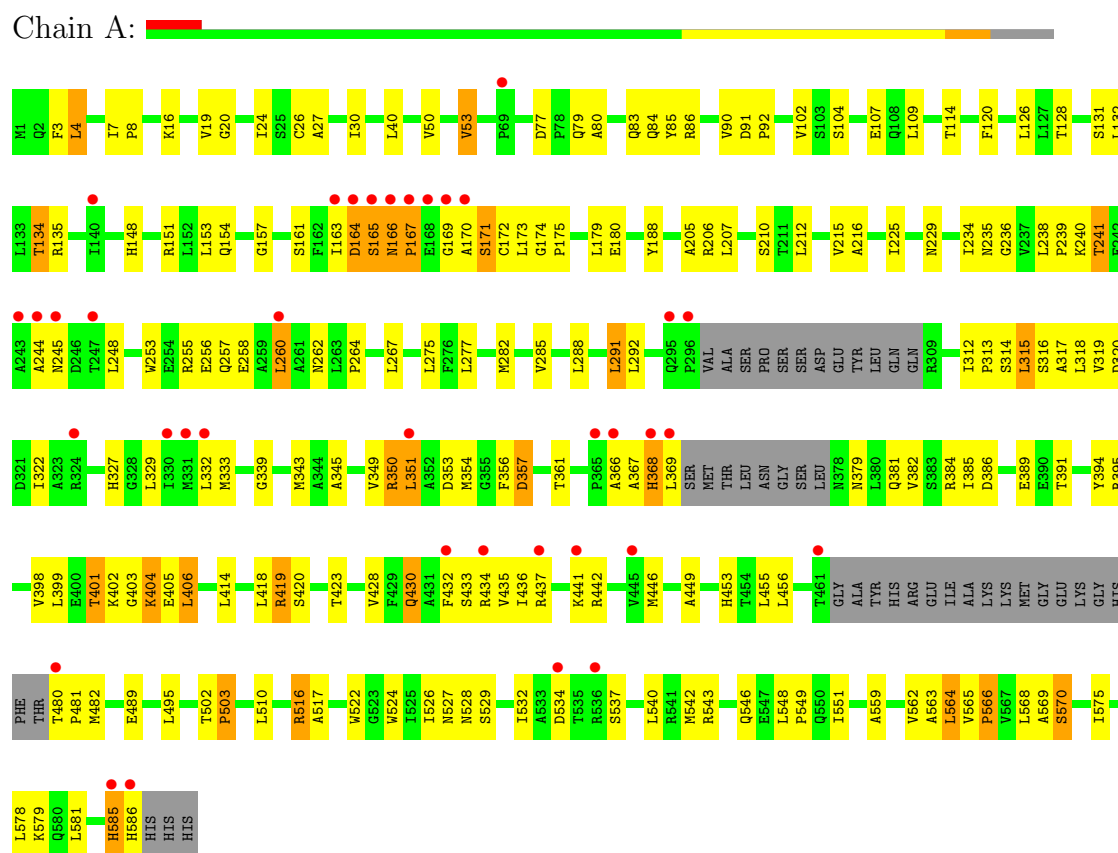
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	217	Total	O	0	0
			217	217		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ARSENITE-TRANSLOCATINGATPASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	73.52Å 75.72Å 222.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.37 – 2.30 26.37 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.4 (26.37-2.30) 93.7 (26.37-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.206 , 0.263 0.201 , 0.259	Depositor DCC
R_{free} test set	2623 reflections (10.98%)	DCC
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.7	EDS
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27783 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4467	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: MG, ADP, CL, CD, SB, SBO

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	0.53	0/4248	0.78	4/5777 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	516	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	171	SER	N-CA-C	5.29	125.30	111.00
1	A	516	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4178	0	4247	176	1
2	A	3	0	0	14	0
3	A	2	0	0	0	0
4	A	6	0	0	0	0
5	A	3	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	4	0	0	4	0
7	A	54	0	24	3	0
8	A	217	0	0	7	1
All	All	4467	0	4271	182	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (182) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:HIS:NE2	2:A:596:SB:SB	2.38	1.35
1:A:453:HIS:NE2	2:A:595:SB:SB	2.41	1.33
1:A:172:CYS:SG	2:A:594:SB:SB	2.69	1.30
2:A:595:SB:SB	5:A:598:CL:CL	2.68	1.29
1:A:420:SER:OG	2:A:596:SB:SB	2.34	1.25
2:A:595:SB:SB	5:A:597:CL:CL	2.82	1.14
2:A:596:SB:SB	8:A:788:HOH:O	2.55	1.04
1:A:367:ALA:HB3	1:A:384:ARG:HH12	1.20	1.04
2:A:595:SB:SB	8:A:720:HOH:O	2.62	0.95
1:A:385:ILE:HD11	1:A:428:VAL:HG13	1.49	0.95
1:A:329:LEU:HD11	1:A:446:MET:HE3	1.48	0.94
1:A:27:ALA:HB1	1:A:292:LEU:HD21	1.54	0.89
1:A:404:LYS:HA	1:A:404:LYS:HE3	1.57	0.87
1:A:381:GLN:NE2	1:A:442:ARG:HH22	1.78	0.82
1:A:368:HIS:ND1	1:A:369:LEU:N	2.30	0.80
1:A:79:GLN:O	1:A:83:GLN:HG3	1.82	0.79
1:A:30:ILE:HD13	1:A:285:VAL:HG13	1.65	0.79
1:A:329:LEU:HD11	1:A:446:MET:CE	2.13	0.79
1:A:369:LEU:HD21	1:A:382:VAL:HG21	1.64	0.78
2:A:594:SB:SB	8:A:717:HOH:O	2.82	0.78
1:A:157:GLY:O	1:A:161:SER:HB2	1.86	0.76
1:A:367:ALA:HB3	1:A:384:ARG:NH1	2.01	0.74
1:A:114:THR:OG1	1:A:175:PRO:HG3	1.87	0.74
1:A:351:LEU:O	1:A:354:MET:HG2	1.90	0.72
1:A:353:ASP:OD1	1:A:579:LYS:HE2	1.90	0.72
1:A:386:ASP:HB3	1:A:389:GLU:HG2	1.73	0.71
1:A:391:THR:O	1:A:395:ARG:HG3	1.91	0.70
1:A:235:ASN:HD22	1:A:275:LEU:HB2	1.56	0.70
1:A:537:SER:OG	1:A:540:LEU:HD23	1.91	0.69
1:A:502:THR:HB	1:A:503:PRO:HD3	1.74	0.69
1:A:148:HIS:CD2	2:A:596:SB:SB	3.27	0.68
1:A:207:LEU:HD13	1:A:256:GLU:HB3	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:238:LEU:HD22	1:A:239:PRO:HD2	1.76	0.67
1:A:128:THR:HG22	1:A:188:TYR:HD1	1.59	0.67
1:A:329:LEU:HD22	1:A:436:ILE:HG23	1.78	0.66
2:A:594:SB:SB	2:A:595:SB:SB	3.74	0.66
1:A:345:ALA:O	1:A:349:VAL:HG23	1.97	0.65
1:A:381:GLN:HE21	1:A:442:ARG:NH2	1.94	0.64
1:A:248:LEU:HD12	1:A:569:ALA:HB2	1.80	0.64
1:A:404:LYS:CA	1:A:404:LYS:HE3	2.28	0.64
1:A:441:LYS:HG3	8:A:895:HOH:O	1.98	0.63
1:A:3:PHE:CE1	1:A:4:LEU:HD13	2.33	0.63
1:A:354:MET:HG3	1:A:356:PHE:CD2	2.34	0.62
1:A:543:ARG:NH2	6:A:701:SBO:SB	3.12	0.62
1:A:369:LEU:HG	1:A:384:ARG:HH22	1.64	0.62
1:A:368:HIS:CG	1:A:369:LEU:N	2.67	0.62
1:A:436:ILE:HG12	1:A:446:MET:CE	2.30	0.62
1:A:207:LEU:HD11	1:A:260:LEU:HD23	1.80	0.62
1:A:319:VAL:CG1	1:A:351:LEU:HD13	2.30	0.61
1:A:430:GLN:CA	1:A:430:GLN:HE21	2.13	0.61
1:A:312:ILE:CD1	1:A:551:ILE:CG2	2.80	0.60
1:A:163:ILE:O	1:A:164:ASP:C	2.40	0.60
1:A:436:ILE:CD1	1:A:446:MET:HE1	2.32	0.60
1:A:83:GLN:HB3	8:A:828:HOH:O	2.01	0.59
1:A:260:LEU:HD13	1:A:260:LEU:O	2.02	0.59
1:A:107:GLU:OE1	1:A:516:ARG:NH2	2.35	0.59
1:A:532:ILE:HG12	1:A:532:ILE:O	2.03	0.59
1:A:16:LYS:HG2	1:A:19:VAL:HG13	1.83	0.59
1:A:381:GLN:NE2	1:A:442:ARG:NH2	2.48	0.59
1:A:240:LYS:HA	1:A:253:TRP:CD1	2.38	0.59
1:A:585:HIS:CG	1:A:586:HIS:H	2.21	0.59
1:A:172:CYS:O	1:A:175:PRO:HD2	2.03	0.58
1:A:529:SER:O	1:A:566:PRO:HA	2.03	0.58
1:A:131:SER:O	1:A:134:THR:HB	2.03	0.58
1:A:432:PHE:O	1:A:436:ILE:HG13	2.03	0.58
1:A:532:ILE:HD12	1:A:564:LEU:HB3	1.86	0.58
1:A:205:ALA:HB2	1:A:215:VAL:HG21	1.85	0.58
1:A:381:GLN:HE21	1:A:442:ARG:HH22	1.46	0.58
1:A:453:HIS:CE1	2:A:595:SB:SB	3.31	0.58
1:A:367:ALA:CB	1:A:384:ARG:HH12	2.06	0.58
1:A:316:SER:OG	1:A:350:ARG:NH2	2.38	0.57
1:A:354:MET:HE2	1:A:356:PHE:HE2	1.68	0.56
1:A:235:ASN:HD21	7:A:590:ADP:HN61	1.52	0.56
1:A:315:LEU:O	1:A:319:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:GLY:HA2	7:A:590:ADP:O1A	2.05	0.56
1:A:345:ALA:HB1	1:A:578:LEU:HD21	1.87	0.56
1:A:568:LEU:HG	1:A:581:LEU:HD23	1.87	0.56
1:A:568:LEU:O	1:A:569:ALA:HB3	2.05	0.56
1:A:314:SER:OG	1:A:316:SER:HB2	2.06	0.56
1:A:166:ASN:HD22	1:A:402:LYS:HE2	1.71	0.56
1:A:225:ILE:O	1:A:225:ILE:HG22	2.05	0.55
1:A:163:ILE:HD12	1:A:173:LEU:HD13	1.88	0.55
1:A:207:LEU:HG	1:A:234:ILE:HG21	1.87	0.55
1:A:170:ALA:HB1	1:A:394:TYR:OH	2.06	0.55
1:A:349:VAL:HG21	1:A:578:LEU:HD23	1.87	0.55
1:A:85:TYR:HE2	1:A:175:PRO:O	1.89	0.54
1:A:248:LEU:CD1	1:A:569:ALA:HB2	2.37	0.54
1:A:394:TYR:O	1:A:398:VAL:HG12	2.07	0.54
1:A:167:PRO:HD2	1:A:402:LYS:HE3	1.90	0.53
1:A:434:ARG:CG	1:A:435:VAL:HG13	2.39	0.53
1:A:357:ASP:OD2	1:A:442:ARG:HD3	2.10	0.52
1:A:354:MET:HG3	1:A:356:PHE:CE2	2.45	0.52
1:A:77:ASP:HB3	1:A:80:ALA:HB3	1.92	0.52
1:A:236:GLY:O	1:A:277:LEU:HB2	2.09	0.52
1:A:436:ILE:HG12	1:A:446:MET:HE1	1.91	0.52
1:A:225:ILE:O	1:A:225:ILE:CG2	2.57	0.51
1:A:174:GLY:N	1:A:175:PRO:CD	2.73	0.51
1:A:128:THR:HG22	1:A:188:TYR:CD1	2.42	0.51
1:A:526:ILE:HB	1:A:564:LEU:HD23	1.93	0.51
1:A:292:LEU:HD22	1:A:292:LEU:N	2.25	0.51
1:A:163:ILE:HD12	1:A:173:LEU:CD1	2.41	0.51
1:A:16:LYS:HG2	1:A:19:VAL:CG1	2.40	0.51
1:A:339:GLY:HA2	7:A:591:ADP:O1A	2.10	0.51
1:A:312:ILE:HD11	1:A:551:ILE:HG22	1.92	0.51
1:A:436:ILE:HG12	1:A:446:MET:HE2	1.93	0.50
1:A:332:LEU:CD2	1:A:343:MET:HB2	2.41	0.50
1:A:86:ARG:HD3	1:A:109:LEU:O	2.11	0.50
1:A:542:MET:O	1:A:546:GLN:HG2	2.10	0.50
1:A:543:ARG:HH21	6:A:701:SBO:SB	2.74	0.50
1:A:532:ILE:HG23	1:A:566:PRO:HB3	1.94	0.50
1:A:120:PHE:CD1	1:A:153:LEU:HD13	2.47	0.50
1:A:50:VAL:O	1:A:53:VAL:HG22	2.12	0.49
1:A:317:ALA:O	1:A:320:ASP:HB2	2.12	0.49
1:A:169:GLY:C	1:A:171:SER:H	2.16	0.49
1:A:264:PRO:HG2	1:A:267:LEU:HD12	1.93	0.49
1:A:26:CYS:HB3	1:A:288:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:453:HIS:CD2	2:A:595:SB:SB	3.40	0.49
1:A:430:GLN:HA	1:A:430:GLN:HE21	1.75	0.48
1:A:430:GLN:O	1:A:433:SER:HB2	2.13	0.48
1:A:568:LEU:C	1:A:569:ALA:O	2.50	0.48
1:A:235:ASN:ND2	1:A:275:LEU:HB2	2.25	0.48
1:A:312:ILE:HD11	1:A:551:ILE:CG2	2.44	0.48
1:A:527:ASN:OD1	1:A:528:ASN:N	2.41	0.48
1:A:292:LEU:HD22	1:A:292:LEU:H	1.78	0.48
1:A:134:THR:HG22	1:A:135:ARG:HG2	1.95	0.48
1:A:434:ARG:O	1:A:437:ARG:HG2	2.14	0.47
1:A:258:GLU:HG2	1:A:262:ASN:HD22	1.79	0.47
1:A:401:THR:HG22	1:A:402:LYS:N	2.29	0.47
1:A:318:LEU:HD22	1:A:522:TRP:CZ3	2.50	0.47
1:A:151:ARG:HA	1:A:154:GLN:HG2	1.97	0.47
1:A:245:ASN:O	1:A:245:ASN:OD1	2.32	0.46
1:A:7:ILE:HG22	1:A:8:PRO:O	2.15	0.46
1:A:434:ARG:HG3	1:A:435:VAL:HG13	1.98	0.46
1:A:206:ARG:NH1	6:A:701:SBO:O3	2.49	0.46
1:A:244:ALA:O	1:A:245:ASN:HB3	2.16	0.46
1:A:235:ASN:ND2	1:A:236:GLY:H	2.14	0.46
1:A:19:VAL:HG11	8:A:795:HOH:O	2.15	0.46
1:A:275:LEU:HD13	1:A:291:LEU:HD22	1.98	0.45
1:A:361:THR:HG21	1:A:435:VAL:HG21	1.98	0.45
1:A:482:MET:HE3	1:A:517:ALA:O	2.16	0.45
1:A:369:LEU:CD2	1:A:382:VAL:HG21	2.40	0.45
1:A:568:LEU:HD23	1:A:568:LEU:HA	1.80	0.45
1:A:418:LEU:O	1:A:423:THR:HG21	2.16	0.45
1:A:529:SER:HB3	1:A:532:ILE:HG22	1.98	0.45
1:A:180:GLU:HA	8:A:734:HOH:O	2.16	0.45
1:A:548:LEU:HB2	1:A:549:PRO:HD3	1.98	0.44
1:A:420:SER:HB3	2:A:594:SB:SB	2.97	0.44
1:A:91:ASP:N	1:A:92:PRO:CD	2.81	0.44
1:A:432:PHE:CD1	1:A:446:MET:SD	3.11	0.44
1:A:404:LYS:HA	1:A:404:LYS:CE	2.40	0.44
1:A:282:MET:SD	1:A:282:MET:N	2.84	0.44
1:A:441:LYS:N	1:A:441:LYS:HD2	2.32	0.44
1:A:318:LEU:O	1:A:322:ILE:HG13	2.18	0.44
1:A:20:GLY:O	1:A:24:ILE:HG13	2.18	0.43
1:A:216:ALA:HA	1:A:267:LEU:HD21	2.00	0.43
1:A:543:ARG:O	1:A:546:GLN:HB2	2.18	0.43
1:A:565:VAL:HG13	1:A:566:PRO:HD2	2.00	0.43
1:A:436:ILE:O	1:A:436:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:333:MET:HG2	1:A:449:ALA:HB3	2.00	0.43
1:A:524:TRP:CG	1:A:559:ALA:HB2	2.54	0.43
1:A:369:LEU:HG	1:A:384:ARG:NH2	2.32	0.43
1:A:354:MET:CE	1:A:356:PHE:HE2	2.30	0.43
1:A:332:LEU:HD23	1:A:343:MET:HB2	2.00	0.43
1:A:564:LEU:HA	1:A:564:LEU:HD23	1.86	0.43
1:A:480:THR:HA	1:A:481:PRO:HD2	1.86	0.42
1:A:436:ILE:CG1	1:A:446:MET:HE1	2.50	0.42
1:A:456:LEU:HD21	1:A:517:ALA:HA	2.00	0.42
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.80	0.42
1:A:404:LYS:HD2	1:A:404:LYS:N	2.35	0.42
1:A:434:ARG:HG2	1:A:435:VAL:HG13	2.02	0.42
1:A:90:VAL:HG13	1:A:102:VAL:HG13	2.02	0.42
1:A:255:ARG:NH1	1:A:570:SER:O	2.49	0.42
1:A:206:ARG:HH22	6:A:701:SBO:SB	2.82	0.41
1:A:318:LEU:HD12	1:A:563:ALA:HB2	2.02	0.41
1:A:240:LYS:HB2	1:A:253:TRP:NE1	2.35	0.41
1:A:403:GLY:HA2	1:A:406:LEU:HD22	2.02	0.41
1:A:404:LYS:O	1:A:405:GLU:HB2	2.20	0.41
1:A:585:HIS:ND1	1:A:586:HIS:N	2.61	0.41
1:A:562:VAL:HG12	1:A:563:ALA:N	2.36	0.41
1:A:312:ILE:HA	1:A:313:PRO:HD3	1.89	0.40
1:A:164:ASP:O	1:A:165:SER:C	2.60	0.40
1:A:240:LYS:O	1:A:241:THR:C	2.58	0.40

All (2) 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	Distance(Å)	Clash(Å)
1:A:240:LYS:NZ	1:A:240:LYS:NZ[2_655]	2.13	0.07
8:A:860:HOH:O	8:A:860:HOH:O[2_655]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	540/589 (92%)	505 (94%)	27 (5%)	8 (2%)	15	13

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	A	164	ASP
1	A	379	ASN
1	A	575	ILE
1	A	166	ASN
1	A	366	ALA
1	A	570	SER
1	A	167	PRO

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	453/487 (93%)	416 (92%)	37 (8%)	17	19

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	40	LEU
1	A	53	VAL
1	A	84	GLN
1	A	104	SER
1	A	126	LEU
1	A	132	LEU
1	A	134	THR
1	A	210	SER
1	A	212	LEU
1	A	229	ASN
1	A	241	THR
1	A	257	GLN
1	A	260	LEU
1	A	291	LEU

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Mol	Chain	Res	Type
1	A	315	LEU
1	A	327	HIS
1	A	350	ARG
1	A	351	LEU
1	A	357	ASP
1	A	368	HIS
1	A	399	LEU
1	A	401	THR
1	A	404	LYS
1	A	406	LEU
1	A	414	LEU
1	A	419	ARG
1	A	430	GLN
1	A	455	LEU
1	A	489	GLU
1	A	495	LEU
1	A	503	PRO
1	A	510	LEU
1	A	534	ASP
1	A	564	LEU
1	A	566	PRO
1	A	585	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	52	GLN
1	A	83	GLN
1	A	138	HIS
1	A	166	ASN
1	A	213	GLN
1	A	229	ASN
1	A	235	ASN
1	A	262	ASN
1	A	327	HIS
1	A	378	ASN
1	A	381	GLN
1	A	430	GLN
1	A	486	GLN
1	A	509	ASN
1	A	586	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 17 ligands modelled in this entry, 14 are monoatomic - leaving 3 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	$\# Z > 2$
7	ADP	A	590	3	29,29,29	1.55	8 (27%)	45,45,45	4.49	22 (48%)
7	ADP	A	591	3	29,29,29	1.48	5 (17%)	45,45,45	4.11	20 (44%)
6	SBO	A	701	-	0,3,3	0.00	-	0,3,3	0.00	-

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
7	ADP	A	590	3	-	0/16/32/32	0/1/3/3
7	ADP	A	591	3	-	0/16/32/32	0/1/3/3
6	SBO	A	701	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	591	ADP	PB-O3A	-3.64	1.53	1.60
7	A	591	ADP	C8-N7	-3.56	1.27	1.34
7	A	590	ADP	C8-N7	-3.38	1.27	1.34
7	A	590	ADP	C8-N9	-3.17	1.31	1.36
7	A	591	ADP	C8-N9	-2.53	1.32	1.36
7	A	590	ADP	PA-O1A	-2.32	1.42	1.51
7	A	590	ADP	C2'-C3'	2.23	1.59	1.53
7	A	591	ADP	O4'-C1'	2.19	1.44	1.41
7	A	591	ADP	C2'-C3'	2.17	1.59	1.53
7	A	590	ADP	PA-O3A	2.16	1.63	1.59
7	A	590	ADP	C2-N3	2.12	1.36	1.32
7	A	590	ADP	C5-C4	-2.09	1.35	1.40
7	A	590	ADP	PB-O2B	-2.03	1.47	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	590	ADP	C4'-O4'-C1'	16.66	127.85	109.75
7	A	591	ADP	C4'-O4'-C1'	14.39	125.38	109.75
7	A	590	ADP	N3-C2-N1	-11.64	118.97	128.71
7	A	590	ADP	O4'-C1'-C2'	-10.67	90.42	106.77
7	A	591	ADP	O4'-C1'-C2'	-9.90	91.59	106.77
7	A	591	ADP	N3-C2-N1	-9.22	121.00	128.71
7	A	590	ADP	C3'-C2'-C1'	8.03	113.48	100.91
7	A	590	ADP	O4'-C1'-N9	-8.01	100.99	108.44
7	A	591	ADP	PA-O3A-PB	7.79	154.52	131.68
7	A	591	ADP	C3'-C2'-C1'	7.28	112.31	100.91
7	A	591	ADP	C5'-C4'-C3'	7.03	143.38	115.21
7	A	591	ADP	O4'-C4'-C5'	-6.65	85.60	109.36
7	A	591	ADP	PA-O5'-C5'	6.33	167.59	122.03
7	A	590	ADP	PA-O5'-C5'	6.25	167.01	122.03
7	A	590	ADP	C5'-C4'-C3'	5.30	136.44	115.21
7	A	590	ADP	C2'-C1'-N9	5.17	126.55	113.27
7	A	590	ADP	C4-C5-N7	-4.82	105.40	109.52
7	A	590	ADP	O2'-C2'-C1'	3.90	123.03	111.23
7	A	591	ADP	O2'-C2'-C1'	3.74	122.55	111.23
7	A	590	ADP	O2A-PA-O1A	3.27	130.46	112.21
7	A	591	ADP	C1'-N9-C4	-3.26	121.01	126.64
7	A	590	ADP	O4'-C4'-C3'	-3.14	98.80	105.17
7	A	590	ADP	C1'-N9-C4	-3.08	121.31	126.64
7	A	590	ADP	O4'-C4'-C5'	-2.96	98.79	109.36
7	A	591	ADP	O4'-C4'-C3'	-2.87	99.34	105.17
7	A	591	ADP	O2A-PA-O1A	2.87	128.26	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	590	ADP	C8-N9-C1'	2.82	131.93	126.38
7	A	590	ADP	C6-C5-N7	2.67	141.54	131.34
7	A	590	ADP	O2A-PA-O3A	2.64	117.65	105.14
7	A	590	ADP	O5'-PA-O1A	-2.63	99.06	109.37
7	A	591	ADP	C2'-C1'-N9	2.40	119.44	113.27
7	A	591	ADP	C2-N1-C6	2.37	123.06	118.77
7	A	591	ADP	O3A-PB-O1B	-2.36	94.87	111.00
7	A	591	ADP	C6-C5-C4	-2.31	113.01	117.25
7	A	591	ADP	O4'-C1'-N9	-2.29	106.31	108.44
7	A	590	ADP	N6-C6-N1	-2.28	114.88	119.36
7	A	590	ADP	C6-C5-C4	-2.28	113.06	117.25
7	A	590	ADP	C2-N3-C4	2.26	120.43	114.01
7	A	591	ADP	O5'-C5'-C4'	-2.20	100.86	108.94
7	A	590	ADP	O3B-PB-O2B	2.18	116.11	107.61
7	A	591	ADP	C8-N9-C4	2.09	108.50	106.90
7	A	591	ADP	O3A-PA-O5'	2.05	112.55	103.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	548/589 (93%)	0.09	37 (6%) 17 25	27, 46, 82, 127	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	ALA	6.6
1	A	165	SER	5.9
1	A	437	ARG	4.1
1	A	445	VAL	4.0
1	A	166	ASN	3.9
1	A	164	ASP	3.9
1	A	295	GLN	3.8
1	A	296	PRO	3.7
1	A	536	ARG	3.7
1	A	167	PRO	3.5
1	A	480	THR	3.4
1	A	244	ALA	3.4
1	A	534	ASP	3.4
1	A	169	GLY	3.4
1	A	168	GLU	3.3
1	A	441	LYS	3.2
1	A	585	HIS	3.2
1	A	245	ASN	3.0
1	A	330	ILE	2.7
1	A	369	LEU	2.6
1	A	365	PRO	2.6
1	A	586	HIS	2.6
1	A	140	ILE	2.5
1	A	324	ARG	2.4
1	A	332	LEU	2.4
1	A	351	LEU	2.4
1	A	331	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	163	ILE	2.4
1	A	461	THR	2.3
1	A	366	ALA	2.3
1	A	432	PHE	2.2
1	A	368	HIS	2.1
1	A	247	THR	2.1
1	A	434	ARG	2.0
1	A	243	ALA	2.0
1	A	260	LEU	2.0
1	A	69	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	SBO	A	701	4/4	0.34	6.84	73,75,78,93	4
3	MG	A	593	1/1	0.18	0.93	34,34,34,34	0
4	CD	A	605	1/1	0.12	0.24	120,120,120,120	1
7	ADP	A	590	27/27	0.12	0.01	30,40,45,46	0
3	MG	A	592	1/1	0.12	-0.28	32,32,32,32	0
2	SB	A	594	1/1	0.09	-0.90	40,40,40,40	0
5	CL	A	598	1/1	0.08	-0.91	31,31,31,31	0
5	CL	A	599	1/1	0.10	-0.93	54,54,54,54	0
4	CD	A	603	1/1	0.14	-0.96	68,68,68,68	1
7	ADP	A	591	27/27	0.10	-0.98	31,41,50,52	0
4	CD	A	601	1/1	0.09	-1.04	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SB	A	595	1/1	0.09	-1.25	36,36,36,36	0
5	CL	A	597	1/1	0.06	-1.30	32,32,32,32	0
4	CD	A	602	1/1	0.09	-1.32	62,62,62,62	0
2	SB	A	596	1/1	0.08	-1.69	39,39,39,39	0
4	CD	A	600	1/1	0.04	-2.94	69,69,69,69	0
4	CD	A	604	1/1	0.06	-8.20	58,58,58,58	1

6.5 Other polymers ⓘ

There are no such residues in this entry.