



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:27 AM UTC

PDB ID : 4AXH / pdb_00004axh
Title : Structure and mechanism of the first inverting alkylsulfatase specific for secondary alkylsulfatases
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Deposited on : 2012-06-13
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

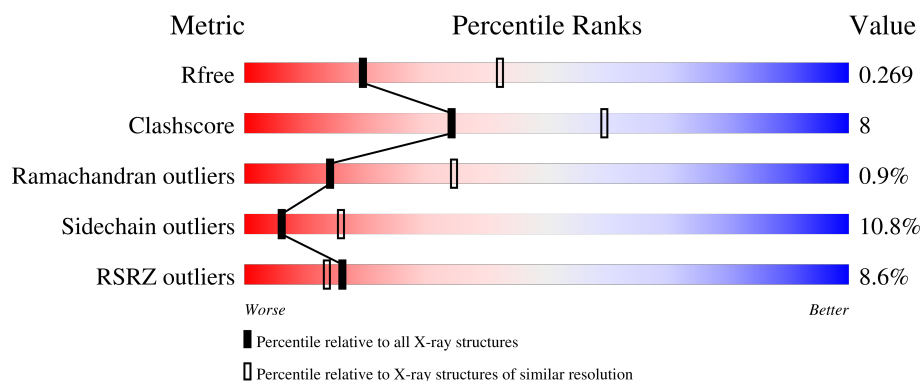
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	668	68% 23% 6%
1	B	668	15% 69% 23% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10045 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 SEC-ALKYLSULFATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	631	Total	C	N	O	S	0	13	0
			4989	3167	867	936	19			
1	B	631	Total	C	N	O	S	0	1	0
			4911	3111	859	922	19			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	661	LEU	-	expression tag	UNP F8KAY7
A	662	GLU	-	expression tag	UNP F8KAY7
A	663	HIS	-	expression tag	UNP F8KAY7
A	664	HIS	-	expression tag	UNP F8KAY7
A	665	HIS	-	expression tag	UNP F8KAY7
A	666	HIS	-	expression tag	UNP F8KAY7
A	667	HIS	-	expression tag	UNP F8KAY7
A	668	HIS	-	expression tag	UNP F8KAY7
A	107	ARG	HIS	conflict	UNP F8KAY7
B	661	LEU	-	expression tag	UNP F8KAY7
B	662	GLU	-	expression tag	UNP F8KAY7
B	663	HIS	-	expression tag	UNP F8KAY7
B	664	HIS	-	expression tag	UNP F8KAY7
B	665	HIS	-	expression tag	UNP F8KAY7
B	666	HIS	-	expression tag	UNP F8KAY7
B	667	HIS	-	expression tag	UNP F8KAY7
B	668	HIS	-	expression tag	UNP F8KAY7
B	107	ARG	HIS	conflict	UNP F8KAY7

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		

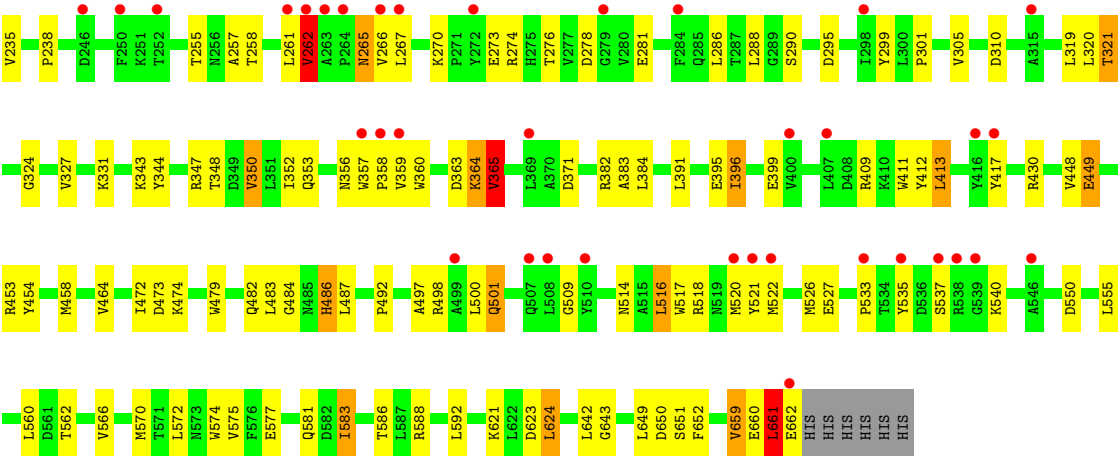
- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total	O	0	0
			98	98		
4	B	38	Total	O	0	0
			38	38		



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.98Å 141.98Å 119.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.59 – 2.70 19.59 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.5 (19.59-2.70) 87.2 (19.59-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.98 (at 2.56Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.221 , 0.266 0.222 , 0.269	Depositor DCC
R_{free} test set	1860 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10045	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, 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	0.94	5/5134 (0.1%)	1.43	33/6960 (0.5%)
1	B	0.87	3/5018 (0.1%)	1.41	31/6808 (0.5%)
All	All	0.91	8/10152 (0.1%)	1.42	64/13768 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	ILE	CA-C	6.15	1.59	1.52
1	A	218	ASN	CG-OD1	5.47	1.33	1.23
1	A	501	GLN	CD-OE1	5.36	1.33	1.23
1	B	93	ASN	CG-OD1	5.27	1.33	1.23
1	B	486	HIS	ND1-CE1	5.25	1.37	1.32
1	A	225	MET	SD-CE	-5.24	1.66	1.79
1	A	93	ASN	CG-OD1	5.22	1.33	1.23
1	B	501	GLN	CD-OE1	5.10	1.33	1.23

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ILE	N-CA-CB	7.65	121.31	111.67
1	A	486	HIS	CB-CG-CD2	-7.56	121.37	131.20
1	A	147	ILE	N-CA-CB	7.53	121.16	111.67
1	B	486	HIS	CB-CG-CD2	-7.53	121.42	131.20
1	A	262	VAL	N-CA-CB	7.21	120.75	111.67
1	B	120	VAL	N-CA-C	-6.91	105.10	111.67
1	A	295	ASP	CA-CB-CG	6.84	119.44	112.60
1	B	295	ASP	CA-CB-CG	6.74	119.34	112.60
1	B	262	VAL	N-CA-CB	6.74	120.16	111.67
1	A	93	ASN	N-CA-C	6.69	119.93	109.96
1	A	319	LEU	N-CA-C	-6.66	105.31	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	ASN	N-CA-C	6.62	119.83	109.96
1	A	120	VAL	N-CA-C	-6.55	105.45	111.67
1	B	650	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	536	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	321	THR	CB-CA-C	6.13	119.20	109.52
1	A	131	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	321	THR	CB-CA-C	6.07	119.10	109.52
1	B	131	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	276	THR	CB-CA-C	5.98	120.65	109.71
1	B	276	THR	CB-CA-C	5.96	120.61	109.71
1	B	97	ALA	N-CA-C	5.84	118.70	110.23
1	B	319	LEU	N-CA-C	-5.74	106.44	113.50
1	A	650	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	219	ILE	CB-CA-C	5.55	116.61	110.62
1	B	139	GLU	CB-CG-CD	5.52	121.99	112.60
1	B	365	VAL	N-CA-CB	5.51	118.85	110.58
1	A	365	VAL	N-CA-CB	5.47	118.78	110.58
1	B	623	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	623	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	396	ILE	N-CA-CB	5.43	117.93	110.54
1	A	147	ILE	CB-CA-C	5.43	118.74	111.19
1	B	147	ILE	CB-CA-C	5.42	118.72	111.19
1	B	224	ALA	CA-C-N	5.36	127.41	120.44
1	B	224	ALA	C-N-CA	5.36	127.41	120.44
1	B	310	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	257	ALA	N-CA-C	5.33	117.37	109.69
1	A	97	ALA	N-CA-C	5.33	117.96	110.23
1	A	523	THR	CA-C-N	5.31	125.84	119.94
1	A	523	THR	C-N-CA	5.31	125.84	119.94
1	B	39	ALA	CA-C-N	5.29	127.33	120.56
1	B	39	ALA	C-N-CA	5.29	127.33	120.56
1	A	658	ILE	CB-CA-C	5.29	116.47	111.44
1	A	145	VAL	N-CA-CB	5.28	118.11	111.46
1	B	643	GLY	CA-C-N	5.25	127.27	120.44
1	B	643	GLY	C-N-CA	5.25	127.27	120.44
1	A	139	GLU	CB-CG-CD	5.22	121.48	112.60
1	B	186	GLY	N-CA-C	5.22	120.21	113.27
1	A	257	ALA	N-CA-C	5.21	117.20	109.69
1	A	224	ALA	CA-C-N	5.20	127.20	120.44
1	A	224	ALA	C-N-CA	5.20	127.20	120.44
1	B	183	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	39	ALA	CA-C-N	5.10	127.08	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ALA	C-N-CA	5.10	127.08	120.56
1	A	220	LEU	N-CA-C	5.09	121.63	110.80
1	B	232	GLN	CA-C-N	5.09	129.28	120.58
1	B	232	GLN	C-N-CA	5.09	129.28	120.58
1	A	643	GLY	CA-C-N	5.06	127.02	120.44
1	A	643	GLY	C-N-CA	5.06	127.02	120.44
1	A	183	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	356	ASN	CA-C-N	5.05	129.12	121.03
1	B	356	ASN	C-N-CA	5.05	129.12	121.03
1	A	186	GLY	N-CA-C	5.03	119.97	113.27
1	B	51	ASN	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	4989	0	4979	80	0
1	B	4911	0	4864	76	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	B	5	0	0	0	0
4	A	98	0	0	12	0
4	B	38	0	0	4	0
All	All	10045	0	9843	150	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 8.

All (150) 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:518:ARG:HA	4:B:2022:HOH:O	1.67	0.95
1:A:527:GLU:HB2	4:A:2054:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:ARG:HH12	1:A:620:ARG:HH21	1.27	0.81
1:A:150:LEU:HB2	4:A:2032:HOH:O	1.82	0.80
1:A:138:ILE:HB	1:A:145:VAL:HG13	1.65	0.79
1:A:605:VAL:HG21	1:A:641:LYS:HB2	1.64	0.78
1:B:138:ILE:HB	1:B:145:VAL:HG13	1.66	0.77
1:A:435:TYR:HE2	1:B:520:MET:HE1	1.49	0.76
1:A:289:GLY:C	4:A:2062:HOH:O	2.30	0.74
1:B:479:TRP:O	1:B:483:LEU:HD12	1.88	0.74
1:A:46:ALA:HA	1:A:49:LEU:HD13	1.70	0.72
1:B:62:ALA:HA	1:B:360:TRP:HZ3	1.52	0.72
1:A:152:THR:O	4:A:2032:HOH:O	2.08	0.72
1:B:449:GLU:O	1:B:453[B]:ARG:HG3	1.88	0.72
1:B:521:TYR:HB2	4:B:2022:HOH:O	1.90	0.71
1:A:524:GLY:HA2	4:A:2054:HOH:O	1.90	0.70
1:A:371:ASP:OD1	1:B:588:ARG:NH2	2.24	0.70
1:B:46:ALA:HA	1:B:49:LEU:HD13	1.73	0.70
1:A:435:TYR:CE2	1:B:520:MET:HE1	2.25	0.70
1:B:238:PRO:HD3	1:B:526:MET:HE1	1.74	0.70
1:A:299:TYR:OH	1:A:347:ARG:HB3	1.95	0.67
1:B:299:TYR:OH	1:B:347:ARG:HB3	1.94	0.67
1:B:54:PHE:H	1:B:411:TRP:HZ2	1.43	0.67
1:B:357:TRP:HE3	1:B:358:PRO:O	1.77	0.67
1:A:258:THR:HG22	1:A:540:LYS:HB3	1.75	0.66
1:B:258:THR:HG22	1:B:540:LYS:HB3	1.75	0.66
1:A:605:VAL:CG2	1:A:641:LYS:HB2	2.25	0.66
1:B:68:ILE:HD11	1:B:119:GLU:HB2	1.77	0.65
1:B:509:GLY:HA2	4:B:2022:HOH:O	1.97	0.65
1:A:391:LEU:HB3	1:A:396:ILE:HG22	1.82	0.62
1:B:147:ILE:HD11	1:B:178:SER:HB3	1.82	0.62
1:A:54:PHE:H	1:A:411:TRP:HZ2	1.47	0.62
1:A:238:PRO:HD3	1:A:526:MET:HE1	1.81	0.62
1:B:391:LEU:HB3	1:B:396:ILE:HG22	1.82	0.62
1:B:65:ARG:HB3	1:B:360:TRP:CH2	2.35	0.61
1:A:147:ILE:HD11	1:A:178:SER:HB3	1.83	0.60
1:A:68:ILE:HD11	1:A:119:GLU:HB2	1.83	0.59
1:A:220:LEU:HG	4:A:2051:HOH:O	2.03	0.58
1:B:357:TRP:CE3	1:B:358:PRO:O	2.56	0.57
1:A:476:ASP:OD2	1:B:453[B]:ARG:NH2	2.37	0.57
1:A:225:MET:HE2	1:A:324:GLY:O	2.05	0.56
1:A:606:THR:HB	1:A:636[A]:ASP:HB3	1.88	0.56
1:A:168:PRO:HG2	1:A:170[A]:LYS:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:TYR:O	1:A:348:THR:HG22	2.07	0.54
1:B:487:LEU:HD23	1:B:497:ALA:HB2	1.90	0.54
1:A:136:THR:HB	1:A:147:ILE:HG23	1.90	0.53
1:B:136:THR:HB	1:B:147:ILE:HG23	1.91	0.53
1:A:101:VAL:HG22	1:A:106[B]:TRP:HD1	1.75	0.52
1:B:352:ILE:HG22	1:B:358:PRO:HB3	1.92	0.52
1:B:350:VAL:HB	1:B:360:TRP:CD1	2.45	0.52
1:B:660:GLU:O	1:B:661:LEU:CB	2.58	0.52
1:B:344:TYR:O	1:B:348:THR:HG22	2.11	0.51
1:A:77[B]:ASN:ND2	1:A:81:GLN:OE1	2.38	0.51
1:A:403:LEU:HD22	4:A:2079:HOH:O	2.09	0.51
1:A:487:LEU:HD23	1:A:497:ALA:HB2	1.93	0.51
1:A:535:TYR:OH	1:A:537:SER:HB2	2.11	0.51
1:A:323:ARG:NH1	4:A:2072:HOH:O	2.43	0.51
1:B:364:LYS:HA	1:B:364:LYS:HE2	1.93	0.51
1:A:454:TYR:HB3	1:A:458:MET:HE2	1.93	0.50
1:B:479:TRP:CD1	1:B:483:LEU:HD11	2.46	0.50
1:A:371:ASP:HB3	1:A:413:LEU:HD21	1.93	0.50
1:A:83:VAL:HA	1:A:255:THR:O	2.11	0.50
1:A:220:LEU:C	1:A:222:GLY:H	2.19	0.50
1:A:624:LEU:HD21	1:A:642:LEU:HD23	1.94	0.50
1:A:353:GLN:HG2	4:A:2068:HOH:O	2.11	0.49
1:A:606:THR:HB	1:A:636[B]:ASP:HB2	1.93	0.49
1:B:83:VAL:HA	1:B:255:THR:O	2.12	0.49
1:A:86:MET:HE1	1:A:113:ASN:HA	1.94	0.49
1:B:86:MET:HE1	1:B:113:ASN:HA	1.95	0.49
1:A:514:ASN:HB3	1:A:517:TRP:HB2	1.95	0.49
1:B:59:GLU:OE2	1:B:357:TRP:HZ2	1.95	0.49
1:A:482:GLN:O	1:A:486:HIS:HD2	1.96	0.49
1:A:270:LYS:HB2	1:A:273:GLU:HG3	1.95	0.49
1:B:535:TYR:OH	1:B:537:SER:HB2	2.13	0.49
1:A:192:ILE:HD11	1:A:262:VAL:HG21	1.95	0.48
1:B:660:GLU:O	1:B:661:LEU:HB2	2.11	0.48
1:B:482:GLN:O	1:B:486:HIS:HD2	1.96	0.48
1:A:352:ILE:HG22	1:A:358:PRO:HB3	1.96	0.48
1:A:391:LEU:HD21	1:A:399:GLU:HG3	1.96	0.47
1:B:454:TYR:HB3	1:B:458:MET:HE2	1.96	0.47
1:A:432:LEU:HD22	1:B:324:GLY:HA3	1.97	0.47
1:B:62:ALA:HA	1:B:360:TRP:CZ3	2.42	0.47
1:A:157:ARG:HH21	1:A:160:LEU:HD23	1.80	0.47
1:B:514:ASN:HB3	1:B:517:TRP:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:HH21	1:B:160:LEU:HD23	1.80	0.47
1:A:157:ARG:NH1	1:A:161:ASP:OD1	2.48	0.47
1:B:270:LYS:HB2	1:B:273:GLU:HG3	1.95	0.47
1:A:433:GLY:HA3	1:B:320:LEU:HD11	1.97	0.46
1:B:391:LEU:HD21	1:B:399:GLU:HG3	1.97	0.46
1:B:357:TRP:HZ3	1:B:359:VAL:HB	1.80	0.46
1:B:624:LEU:HD21	1:B:642:LEU:HD23	1.97	0.46
1:B:353:GLN:HG2	4:B:2016:HOH:O	2.14	0.46
1:A:286:LEU:HD22	1:A:288:LEU:HD21	1.97	0.46
1:B:192:ILE:HD11	1:B:262:VAL:HG21	1.97	0.46
1:A:101:VAL:CG2	1:A:106[B]:TRP:HD1	2.29	0.45
1:A:412:TYR:CD1	1:A:413:LEU:HD13	2.52	0.45
1:A:40:ILE:H	1:A:40:ILE:HD12	1.80	0.45
1:A:482:GLN:O	1:A:486:HIS:CD2	2.69	0.45
1:B:570:MET:SD	1:B:572:LEU:HD11	2.56	0.45
1:B:574:TRP:HB2	1:B:583:ILE:HG23	1.99	0.44
1:A:233:SER:HA	4:A:2055:HOH:O	2.16	0.44
1:A:348:THR:HG23	1:A:365:VAL:HG21	1.99	0.44
1:B:204:VAL:H	1:B:265:ASN:HB2	1.82	0.44
1:A:417:TYR:O	1:A:516:LEU:HD22	2.17	0.44
1:B:371:ASP:HB3	1:B:413:LEU:HD21	1.98	0.44
1:B:417:TYR:O	1:B:516:LEU:HD22	2.17	0.44
1:A:274[A]:ARG:HH12	1:A:301:PRO:HG3	1.82	0.44
1:B:231:TYR:OH	1:B:659:VAL:HG23	2.18	0.44
1:A:204:VAL:H	1:A:265:ASN:HB2	1.82	0.44
1:B:484:GLY:HA3	1:B:501:GLN:HG3	1.98	0.44
1:A:274[A]:ARG:NH2	1:A:281:GLU:OE1	2.51	0.44
1:B:482:GLN:O	1:B:486:HIS:CD2	2.71	0.44
1:B:65:ARG:HB3	1:B:360:TRP:CZ3	2.53	0.44
1:A:574:TRP:HB2	1:A:583:ILE:HG23	1.99	0.43
1:B:562:THR:O	1:B:566:VAL:HG23	2.19	0.43
1:B:492:PRO:O	1:B:498:ARG:HD2	2.18	0.43
1:A:383:ALA:HA	1:A:396:ILE:HD12	2.00	0.43
1:B:227:ARG:HH22	1:B:527:GLU:CD	2.27	0.43
1:B:464:VAL:HG23	1:B:487:LEU:HD22	1.99	0.43
1:B:479:TRP:NE1	1:B:483:LEU:HD11	2.33	0.43
1:B:286:LEU:HD22	1:B:288:LEU:HD21	1.99	0.43
1:A:143:GLY:HA3	1:A:173:VAL:HG23	2.01	0.43
1:A:484:GLY:HA3	1:A:501:GLN:HG3	1.99	0.43
1:A:375:MET:HA	4:A:2079:HOH:O	2.17	0.43
1:A:570:MET:SD	1:A:572:LEU:HD11	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:H	1:B:40:ILE:HD12	1.84	0.43
1:A:464:VAL:HG23	1:A:487:LEU:HD22	2.01	0.42
1:B:383:ALA:HA	1:B:396:ILE:HD12	2.01	0.42
1:A:189:ARG:NE	4:A:2042:HOH:O	2.19	0.42
1:B:157:ARG:NH1	1:B:161:ASP:OD1	2.52	0.42
1:B:281:GLU:HB3	1:B:301:PRO:HG2	2.02	0.42
1:B:143:GLY:HA3	1:B:173:VAL:HG23	2.02	0.42
1:B:348:THR:HG23	1:B:365:VAL:HG21	2.01	0.42
1:B:357:TRP:CZ3	1:B:359:VAL:HB	2.55	0.42
1:A:101:VAL:HG13	1:A:106[B]:TRP:CD1	2.55	0.42
1:A:492:PRO:O	1:A:498:ARG:HD2	2.20	0.42
1:A:562:THR:O	1:A:566:VAL:HG23	2.19	0.42
1:A:518:ARG:O	1:A:522:MET:HB2	2.20	0.42
1:A:227:ARG:HH22	1:A:527:GLU:CD	2.28	0.41
1:B:223:THR:HG21	1:B:652:PHE:HB2	2.02	0.41
1:A:142:SER:H	1:A:278:ASP:CG	2.28	0.41
1:B:412:TYR:CD1	1:B:413:LEU:HD13	2.54	0.41
1:B:142:SER:H	1:B:278:ASP:CG	2.28	0.41
1:A:169[A]:LYS:HD2	1:A:169[A]:LYS:HA	1.74	0.41
1:A:560:LEU:HD22	1:A:592:LEU:HB2	2.03	0.41
1:A:300:LEU:HD12	1:A:305:VAL:CG2	2.51	0.41
1:A:321:THR:HA	1:A:322:PRO:HD3	1.97	0.40
1:B:560:LEU:HD22	1:B:592:LEU:HB2	2.02	0.40
1:B:65:ARG:HD3	1:B:360:TRP:CZ3	2.56	0.40
1:B:213:HIS:O	1:B:217:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	642/668 (96%)	602 (94%)	34 (5%)	6 (1%)	14 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	630/668 (94%)	591 (94%)	34 (5%)	5 (1%)	16	37
All	All	1272/1336 (95%)	1193 (94%)	68 (5%)	11 (1%)	14	35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	GLU
1	A	220	LEU
1	B	661	LEU
1	A	290	SER
1	A	533	PRO
1	B	139	GLU
1	B	290	SER
1	B	533	PRO
1	A	53	PRO
1	B	53	PRO
1	A	221	ALA

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	522/539 (97%)	469 (90%)	53 (10%)	7	18
1	B	508/539 (94%)	450 (89%)	58 (11%)	5	14
All	All	1030/1078 (96%)	919 (89%)	111 (11%)	6	16

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

Mol	Chain	Res	Type
1	A	52	LEU
1	A	72	SER
1	A	76	LYS
1	A	90	GLN
1	A	101	VAL

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Mol	Chain	Res	Type
1	A	145	VAL
1	A	147	ILE
1	A	160	LEU
1	A	169[A]	LYS
1	A	169[B]	LYS
1	A	182	ILE
1	A	223	THR
1	A	225	MET
1	A	235	VAL
1	A	236	MET
1	A	261	LEU
1	A	262	VAL
1	A	265	ASN
1	A	266	VAL
1	A	267	LEU
1	A	305	VAL
1	A	321	THR
1	A	323	ARG
1	A	327	VAL
1	A	331	LYS
1	A	343	LYS
1	A	350	VAL
1	A	365	VAL
1	A	382	ARG
1	A	384	LEU
1	A	395	GLU
1	A	396	ILE
1	A	413	LEU
1	A	430	ARG
1	A	448	VAL
1	A	449	GLU
1	A	472	ILE
1	A	473	ASP
1	A	500	LEU
1	A	522	MET
1	A	536	ASP
1	A	550	ASP
1	A	555	LEU
1	A	575	VAL
1	A	577	GLU
1	A	581	GLN
1	A	583	ILE

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Mol	Chain	Res	Type
1	A	586	THR
1	A	605	VAL
1	A	621	LYS
1	A	624	LEU
1	A	649	LEU
1	A	651	SER
1	B	52	LEU
1	B	72	SER
1	B	76	LYS
1	B	90	GLN
1	B	101	VAL
1	B	106	TRP
1	B	145	VAL
1	B	147	ILE
1	B	160	LEU
1	B	182	ILE
1	B	212	GLU
1	B	219	ILE
1	B	223	THR
1	B	235	VAL
1	B	261	LEU
1	B	262	VAL
1	B	265	ASN
1	B	266	VAL
1	B	267	LEU
1	B	274	ARG
1	B	305	VAL
1	B	321	THR
1	B	327	VAL
1	B	331	LYS
1	B	343	LYS
1	B	350	VAL
1	B	363	ASP
1	B	364	LYS
1	B	365	VAL
1	B	382	ARG
1	B	384	LEU
1	B	395	GLU
1	B	396	ILE
1	B	409	ARG
1	B	413	LEU
1	B	430	ARG

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Mol	Chain	Res	Type
1	B	448	VAL
1	B	449	GLU
1	B	472	ILE
1	B	473	ASP
1	B	474	LYS
1	B	500	LEU
1	B	516	LEU
1	B	522	MET
1	B	550	ASP
1	B	555	LEU
1	B	575	VAL
1	B	577	GLU
1	B	581	GLN
1	B	583	ILE
1	B	586	THR
1	B	621	LYS
1	B	624	LEU
1	B	649	LEU
1	B	651	SER
1	B	659	VAL
1	B	661	LEU
1	B	662	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	ASN
1	A	388	ASN
1	A	441	ASN
1	A	494	ASN
1	A	657	ASN
1	B	311	ASN
1	B	356	ASN
1	B	388	ASN
1	B	441	ASN
1	B	494	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	SO4	B	800	-	4,4,4	0.35	0	6,6,6	0.47	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	631/668 (94%)	-0.16	9 (1%) 73 72	14, 45, 105, 139	13 (2%)
1	B	631/668 (94%)	0.88	100 (15%) 5 4	29, 101, 159, 173	1 (0%)
All	All	1262/1336 (94%)	0.36	109 (8%) 16 13	14, 70, 152, 173	14 (1%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	ASN	4.2
1	B	163	TYR	4.0
1	A	219	ILE	4.0
1	B	197	VAL	4.0
1	B	214	ALA	3.8
1	B	105	LEU	3.7
1	B	205	PHE	3.7
1	B	138	ILE	3.6
1	B	127	VAL	3.4
1	B	180	SER	3.3
1	B	137	ILE	3.2
1	B	68	ILE	3.2
1	B	117	LEU	3.2
1	B	75	ILE	3.1
1	B	159	ALA	3.1
1	B	359	VAL	3.1
1	B	400	VAL	3.1
1	B	358	PRO	3.0
1	B	357	TRP	3.0
1	B	538	ARG	3.0
1	B	172	ILE	2.9
1	B	250	PHE	2.9
1	B	508	LEU	2.8
1	B	263	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	120	VAL	2.8
1	B	145	VAL	2.7
1	B	160	LEU	2.7
1	B	63	ALA	2.7
1	B	211	MET	2.7
1	B	141	ASP	2.7
1	B	134	ASN	2.7
1	B	264	PRO	2.7
1	B	416	TYR	2.6
1	B	267	LEU	2.6
1	A	221	ALA	2.6
1	B	162	LEU	2.6
1	B	662	GLU	2.6
1	A	220	LEU	2.5
1	B	204	VAL	2.5
1	B	88	ALA	2.5
1	B	298	ILE	2.5
1	B	261	LEU	2.5
1	B	129	GLY	2.5
1	B	147	ILE	2.5
1	B	407	LEU	2.5
1	B	53	PRO	2.5
1	B	82	VAL	2.5
1	B	266	VAL	2.5
1	B	252	THR	2.5
1	B	52	LEU	2.5
1	B	54	PHE	2.5
1	B	210	PHE	2.5
1	B	122	PRO	2.4
1	B	48	VAL	2.4
1	B	177	TYR	2.4
1	B	60	PHE	2.4
1	B	84	TRP	2.3
1	B	126	GLN	2.3
1	B	533	PRO	2.3
1	A	539	GLY	2.3
1	B	192	ILE	2.3
1	B	535	TYR	2.3
1	B	133	ALA	2.2
1	B	125	TYR	2.2
1	B	417	TYR	2.2
1	B	67	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	92	LEU	2.2
1	B	55	ALA	2.2
1	B	123	LYS	2.2
1	B	136	THR	2.2
1	B	89	TYR	2.2
1	B	507	GLN	2.2
1	B	262	VAL	2.2
1	B	521	TYR	2.2
1	B	246	ASP	2.2
1	B	546	ALA	2.2
1	B	369	LEU	2.2
1	B	522	MET	2.2
1	B	315	ALA	2.1
1	B	70	PRO	2.1
1	B	103	PRO	2.1
1	B	537	SER	2.1
1	B	100	THR	2.1
1	B	140	GLY	2.1
1	B	539	GLY	2.1
1	A	537	SER	2.1
1	B	499	ALA	2.1
1	B	106	TRP	2.1
1	B	108	GLN	2.1
1	B	520	MET	2.1
1	B	32	LEU	2.1
1	B	124	LEU	2.1
1	B	45	ASN	2.1
1	B	284	PHE	2.1
1	B	38	SER	2.1
1	B	98	ALA	2.1
1	B	152	THR	2.1
1	A	622	LEU	2.1
1	A	635	LEU	2.1
1	B	130	LEU	2.1
1	B	114	ILE	2.1
1	B	176	VAL	2.1
1	B	279	GLY	2.0
1	B	272	TYR	2.0
1	B	37	ALA	2.0
1	A	567	GLY	2.0
1	B	51	ASN	2.0
1	B	202	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	510	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	800	5/5	0.88	0.12	81,84,86,87	0
2	ZN	B	701	1/1	0.96	0.05	89,89,89,89	0
2	ZN	B	700	1/1	0.97	0.05	104,104,104,104	0
2	ZN	A	701	1/1	0.99	0.02	39,39,39,39	0
2	ZN	A	700	1/1	1.00	0.02	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.