Full wwPDB X-ray Structure Validation Report

Apr 29, 2024 – 03:35 am BST

PDB ID	:	4AXH
Title	:	Structure and mechanism of the first inverting alkylsulfatase specific for secondary alkylsulfatases
Authors	:	Knaus, T.; Schober, M.; Faber, K.; Macheroux, P.; Wagner, U.G.
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:

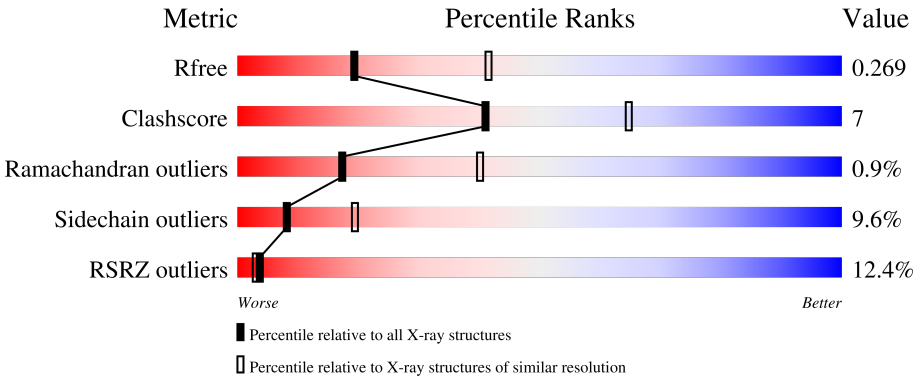
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	3% 72% 20% · 6%
1	B	668	20% 73% 20% · 6%

2 Entry composition (i)

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 (three-letter code: ZN) (formula: Zn).

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

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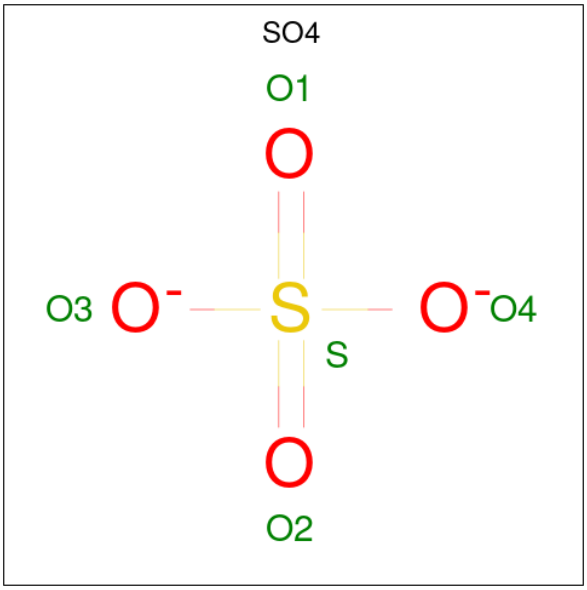
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Zn 2 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

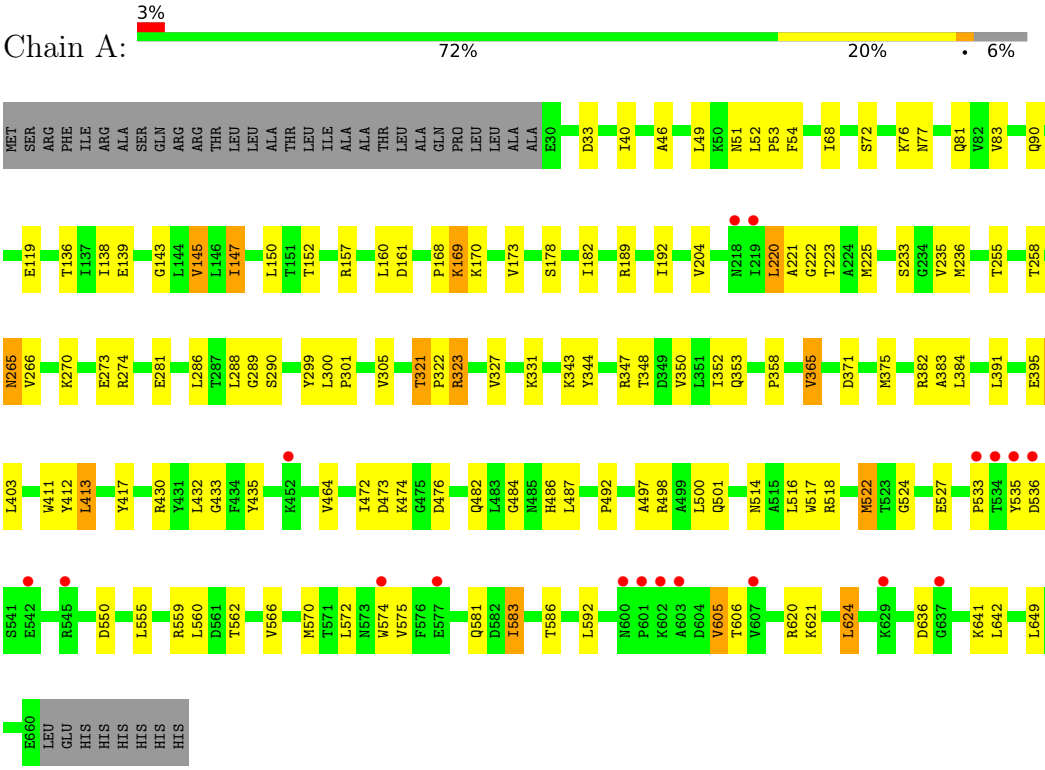
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	98	Total O 98 98	0	0
4	B	38	Total O 38 38	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

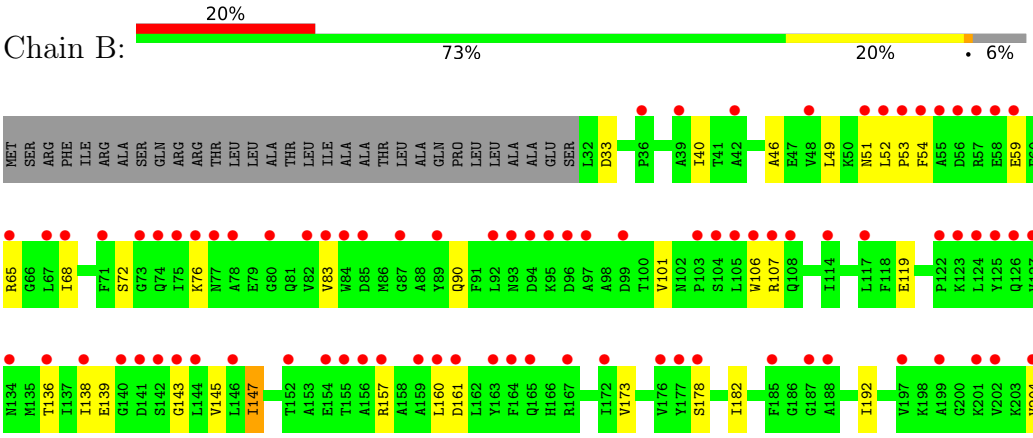
• Molecule 1: SEC-ALKYLSULFATASE

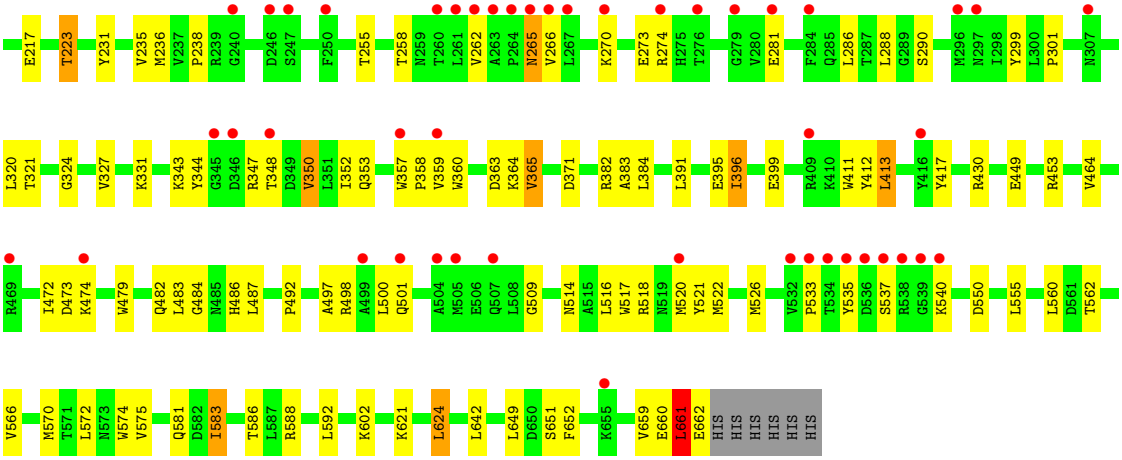
Chain A:



• Molecule 1: SEC-ALKYLSULFATASE

Chain B:




E217 T223 Y231 V235 M236 V237 P238 R239 G240 D246 S247 F250 T255 T258 N259 T260 L261 V262 A263 P264 N265 V266 L267 K270 E273 R274 H275 T276 G279 V280 E281 F284 Q285 L286 T287 L288 G289 S290 M296 N297 I298 Y299 L300 P301 N307
L320 T321 G324 V327 K331 K343 Y344 G345 D346 R347 T348 D349 V350 L351 I352 Q353 W357 P358 V359 W360 D363 K364 V365 D371 R382 A383 L384 L391 E395 I396 E399 R409 K410 W411 Y412 L413 Y416 Y417 R430 E449 R453 V464
R469 I472 D473 K474 W479 Q482 L483 G484 N485 H486 L487 P492 A497 R498 A499 L500 Q501 A504 M505 E506 Q507 L508 G509 N514 A515 L516 W517 R518 N519 M520 Y521 M522 M526 V532 P533 T534 Y535 D536 S537 R538 G539 K540 D550 L555 L560 D561 T562
V566 M570 T571 L572 N573 W574 V575 Q581 D582 I583 T586 L587 R588 L592 K602 K621 L624 L642 L649 D650 S651 F652 K655 V659 E660 L661 E662 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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 19.93 – 2.54	Depositor EDS
% Data completeness (in resolution range)	93.5 (19.59-2.70) 80.4 (19.93-2.54)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 70.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o,F_c correlation	0.84	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, ZN

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	0.58	0/5134	0.76	0/6960
1	B	0.52	0/5018	0.75	0/6808
All	All	0.55	0/10152	0.76	0/13768

There are no bond length outliers.

There are no bond angle outliers.

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	74	0
1	B	4911	0	4864	73	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	141	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 (141) 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
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	0.74
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:289:GLY:C	4:A:2062:HOH:O	2.30	0.69
1:A:435:TYR:CE2	1:B:520:MET:HE1	2.28	0.67
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: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: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:B:299:TYR:HH	1:B:347:ARG:HB3	1.76	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:220:LEU:C	1:A:222:GLY:H	2.19	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:238:PRO:HD3	1:B:526:MET:HE1	1.98	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:223:THR:HG21	1:B:652:PHE:HB2	2.02	0.41
1:B:412:TYR:CD1	1:B:413:LEU:HD13	2.54	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 (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	642/668 (96%)	602 (94%)	34 (5%)	6 (1%)	17	40
1	B	630/668 (94%)	591 (94%)	34 (5%)	5 (1%)	19	43
All	All	1272/1336 (95%)	1193 (94%)	68 (5%)	11 (1%)	17	40

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 (i)

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%)	472 (90%)	50 (10%)	8 19
1	B	508/539 (94%)	459 (90%)	49 (10%)	8 19
All	All	1030/1078 (96%)	931 (90%)	99 (10%)	8 19

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	51	ASN
1	A	52	LEU
1	A	72	SER
1	A	76	LYS
1	A	90	GLN
1	A	101	VAL
1	A	145	VAL
1	A	147	ILE
1	A	169[A]	LYS
1	A	169[B]	LYS
1	A	182	ILE
1	A	223	THR

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Mol	Chain	Res	Type
1	A	225	MET
1	A	235	VAL
1	A	236	MET
1	A	261	LEU
1	A	265	ASN
1	A	266	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	472	ILE
1	A	473	ASP
1	A	474	LYS
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	581	GLN
1	A	583	ILE
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	A	655	LYS
1	B	33	ASP
1	B	51	ASN
1	B	52	LEU
1	B	72	SER
1	B	76	LYS

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Mol	Chain	Res	Type
1	B	90	GLN
1	B	101	VAL
1	B	106	TRP
1	B	107	ARG
1	B	147	ILE
1	B	182	ILE
1	B	212	GLU
1	B	223	THR
1	B	235	VAL
1	B	236	MET
1	B	265	ASN
1	B	266	VAL
1	B	274	ARG
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	365	VAL
1	B	382	ARG
1	B	384	LEU
1	B	395	GLU
1	B	396	ILE
1	B	413	LEU
1	B	430	ARG
1	B	472	ILE
1	B	473	ASP
1	B	474	LYS
1	B	500	LEU
1	B	522	MET
1	B	550	ASP
1	B	555	LEU
1	B	575	VAL
1	B	581	GLN
1	B	583	ILE
1	B	586	THR
1	B	602	LYS
1	B	621	LYS
1	B	624	LEU
1	B	649	LEU
1	B	651	SER

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Mol	Chain	Res	Type
1	B	661	LEU
1	B	662	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

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	0.25	0	6,6,6	0.58	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, 95^{th} 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%)	-0.29	21 (3%) 46 46	23, 45, 105, 139	0
1	B	631/668 (94%)	0.96	135 (21%) 0 0	32, 101, 159, 173	0
All	All	1262/1336 (94%)	0.33	156 (12%) 4 3	23, 70, 152, 173	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	537	SER	9.2
1	A	539	GLY	8.3
1	B	51	ASN	8.1
1	B	199	ALA	7.0
1	A	218	ASN	6.4
1	B	536	ASP	6.4
1	B	279	GLY	6.3
1	B	535	TYR	6.1
1	B	54	PHE	6.1
1	B	539	GLY	6.1
1	A	538	ARG	5.7
1	A	219	ILE	5.7
1	B	533	PRO	5.4
1	B	163	TYR	5.4
1	B	177	TYR	5.3
1	B	197	VAL	5.2
1	B	68	ILE	5.1
1	A	536	ASP	4.8
1	B	141	ASP	4.6
1	B	125	TYR	4.5
1	A	537	SER	4.5
1	A	601	PRO	4.4
1	B	538	ARG	4.4
1	B	266	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	297	ASN	4.3
1	B	205	PHE	4.3
1	B	53	PRO	4.2
1	B	140	GLY	4.2
1	B	270	LYS	4.2
1	B	122	PRO	4.2
1	B	71	PHE	4.1
1	B	85	ASP	4.0
1	A	629	LYS	3.9
1	A	535	TYR	3.9
1	B	52	LEU	3.9
1	B	78	ALA	3.8
1	B	143	GLY	3.8
1	B	187	GLY	3.8
1	B	82	VAL	3.8
1	B	117	LEU	3.7
1	A	542	GLU	3.7
1	B	160	LEU	3.7
1	B	76	LYS	3.6
1	B	263	ALA	3.6
1	B	202	VAL	3.6
1	B	159	ALA	3.5
1	B	96	ASP	3.5
1	B	161	ASP	3.5
1	B	129	GLY	3.4
1	B	167	ARG	3.4
1	B	281	GLU	3.4
1	B	89	TYR	3.3
1	B	204	VAL	3.3
1	B	106	TRP	3.3
1	B	346	ASP	3.3
1	B	142	SER	3.3
1	B	296	MET	3.2
1	B	103	PRO	3.2
1	B	124	LEU	3.2
1	A	545	ARG	3.2
1	B	39	ALA	3.2
1	B	126	GLN	3.1
1	B	154	GLU	3.1
1	B	80	GLY	3.0
1	B	201	LYS	3.0
1	B	136	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	94	ASP	3.0
1	B	56	ASP	3.0
1	B	240	GLY	3.0
1	B	92	LEU	3.0
1	A	533	PRO	3.0
1	B	250	PHE	2.9
1	B	97	ALA	2.9
1	B	93	ASN	2.9
1	B	265	ASN	2.9
1	B	75	ILE	2.9
1	B	165	GLN	2.9
1	B	176	VAL	2.9
1	B	357	TRP	2.8
1	B	152	THR	2.8
1	B	146	LEU	2.8
1	B	172	ILE	2.8
1	B	274	ARG	2.8
1	B	246	ASP	2.8
1	B	284	PHE	2.8
1	B	57	ARG	2.8
1	B	59	GLU	2.8
1	B	130	LEU	2.7
1	B	188	ALA	2.7
1	B	73	GLY	2.7
1	B	48	VAL	2.7
1	B	655	LYS	2.7
1	B	127	VAL	2.7
1	B	507	GLN	2.7
1	B	359	VAL	2.6
1	B	36	PRO	2.6
1	B	138	ILE	2.6
1	B	55	ALA	2.6
1	B	416	TYR	2.6
1	A	600	ASN	2.5
1	B	474	LYS	2.5
1	B	105	LEU	2.5
1	B	123	LYS	2.5
1	B	164	PHE	2.5
1	B	276	THR	2.5
1	A	607	VAL	2.5
1	B	61	GLU	2.5
1	B	156	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	104	SER	2.4
1	B	534	THR	2.4
1	B	501	GLN	2.4
1	A	534	THR	2.4
1	B	532	VAL	2.4
1	B	63	ALA	2.4
1	B	99	ASP	2.4
1	B	83	VAL	2.3
1	B	409	ARG	2.3
1	B	264	PRO	2.3
1	B	65	ARG	2.3
1	A	574	TRP	2.3
1	B	107	ARG	2.3
1	B	157	ARG	2.3
1	B	114	ILE	2.3
1	B	262	VAL	2.3
1	B	155	THR	2.3
1	A	452	LYS	2.3
1	B	87	GLY	2.2
1	B	84	TRP	2.2
1	B	307	ASN	2.2
1	A	637	GLY	2.2
1	B	267	LEU	2.2
1	B	134	ASN	2.2
1	B	58	GLU	2.2
1	B	540	LYS	2.2
1	B	67	LEU	2.2
1	B	42	ALA	2.2
1	B	499	ALA	2.2
1	B	505	MET	2.2
1	B	348	THR	2.2
1	A	602	LYS	2.1
1	B	77	ASN	2.1
1	B	345	GLY	2.1
1	B	504	ALA	2.1
1	B	520	MET	2.1
1	B	185	PHE	2.1
1	B	260	THR	2.1
1	A	577	GLU	2.1
1	B	95	LYS	2.1
1	B	178	SER	2.1
1	B	261	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	74	GLN	2.1
1	B	108	GLN	2.1
1	A	603	ALA	2.1
1	B	144	LEU	2.0
1	B	469	ARG	2.0
1	B	247	SER	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 monosaccharides 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, 95^{th} 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
2	ZN	B	701	1/1	0.94	0.04	89,89,89,89	0
3	SO4	B	800	5/5	0.94	0.18	81,84,86,87	0
2	ZN	B	700	1/1	0.97	0.04	104,104,104,104	0
2	ZN	A	701	1/1	0.99	0.03	39,39,39,39	0
2	ZN	A	700	1/1	0.99	0.03	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.