



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:27 AM UTC

PDB ID : 4P04 / pdb_00004p04
Title : Apo form of bacterial arylsulfate sulfotransferase (ASST) H436N mutant with MPO in the active site
Authors : Malojcic, G.; Owen, R.L.; Glockshuber, R.
Deposited on : 2014-02-20
Resolution : 1.95 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

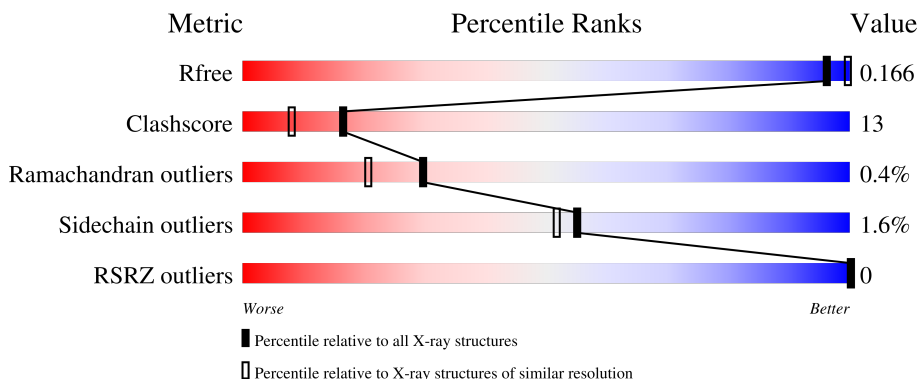
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	571	 75% 23% ..
1	B	571	 74% 24% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9763 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.

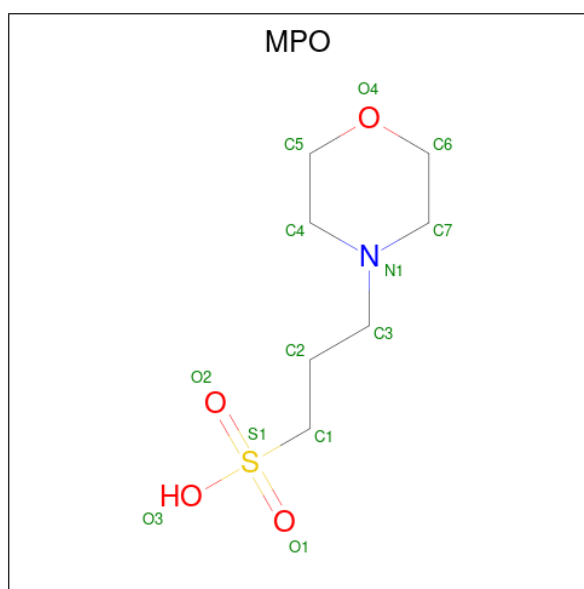
- Molecule 1 is a protein called Arylsulfate sulfotransferase AssT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	567	Total	C	N	O	S	0	2	0
			4472	2840	768	854	10			
1	B	563	Total	C	N	O	S	0	3	0
			4450	2827	761	852	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	ASN	HIS	engineered mutation	UNP E2QE64
B	436	ASN	HIS	engineered mutation	UNP E2QE64

- Molecule 2 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- 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		

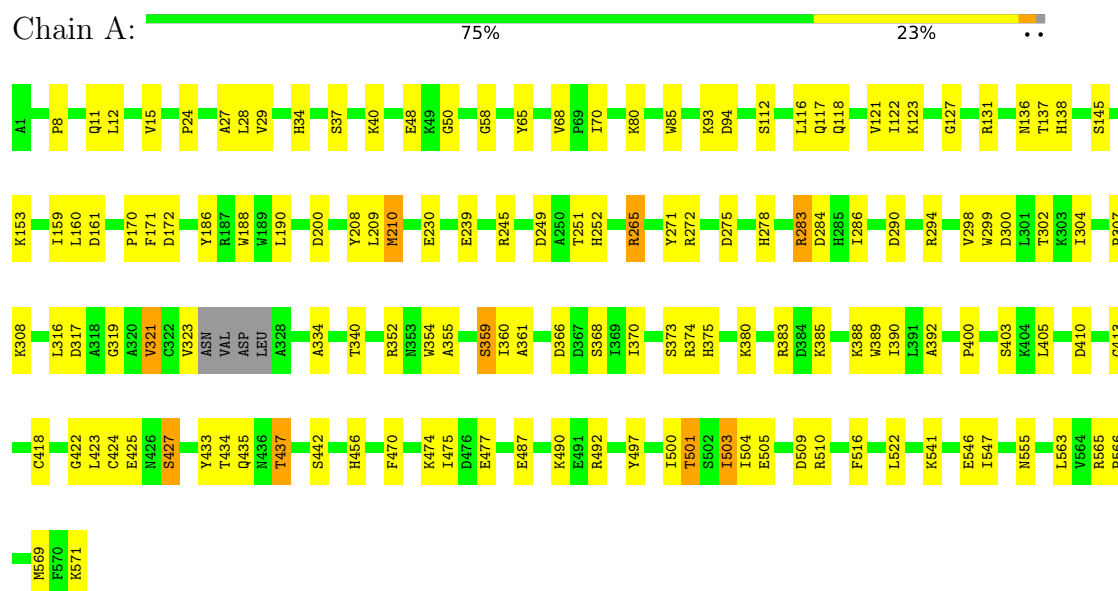
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	411	Total	O	0	0
			411	411		
4	B	399	Total	O	0	0
			399	399		

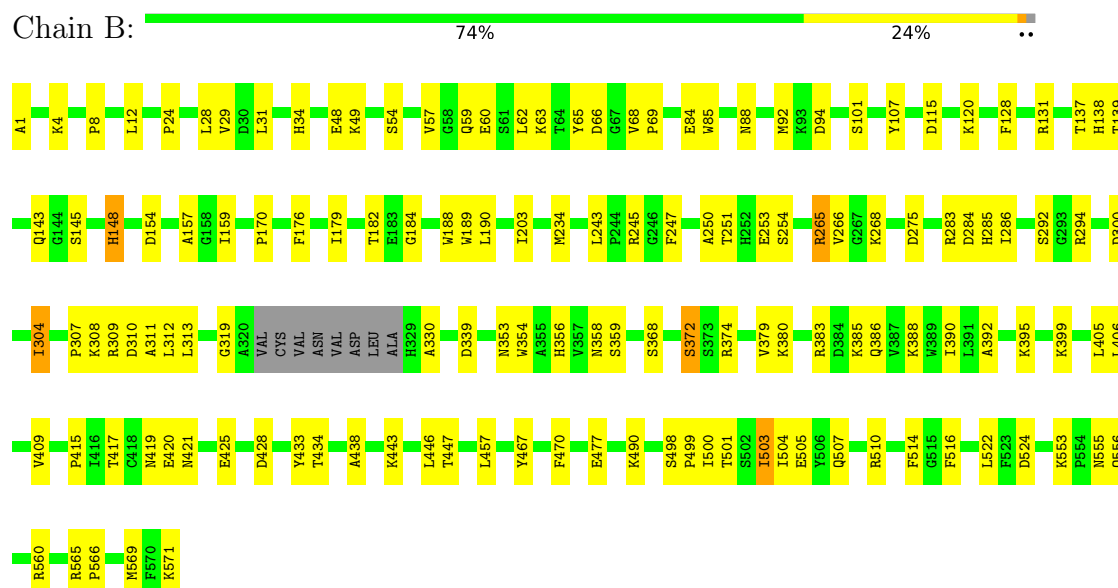
3 Residue-property plots

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

• Molecule 1: Arylsulfate sulfotransferase AssT



• Molecule 1: Arylsulfate sulfotransferase AssT



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	181.49Å 181.49Å 99.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.02 – 1.95 51.02 – 1.95	Depositor EDS
% Data completeness (in resolution range)	90.8 (51.02-1.95) 90.8 (51.02-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309), REFMAC	Depositor
R, R_{free}	0.150 , 0.167 0.154 , 0.166	Depositor DCC
R_{free} test set	6188 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.449 for -h,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9763	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: MPO, 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	0.63	0/4587	0.87	7/6223 (0.1%)
1	B	0.60	1/4568 (0.0%)	0.83	3/6199 (0.0%)
All	All	0.61	1/9155 (0.0%)	0.85	10/12422 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	286	ILE	CA-CB	-5.24	1.48	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	NE-CZ-NH2	6.08	124.68	119.20
1	B	565	ARG	CA-C-N	5.98	126.41	119.47
1	B	565	ARG	C-N-CA	5.98	126.41	119.47
1	A	565	ARG	CA-C-N	5.75	125.42	119.56
1	A	565	ARG	C-N-CA	5.75	125.42	119.56
1	A	210	MET	N-CA-C	5.60	115.50	108.45
1	A	265	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	A	37	SER	N-CA-C	5.20	120.10	113.18
1	A	283	ARG	N-CA-C	5.19	118.36	111.30
1	B	470	PHE	N-CA-C	-5.08	101.42	109.96

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	4472	0	4332	115	0
1	B	4450	0	4302	113	1
2	A	13	0	15	5	0
2	B	13	0	15	5	0
3	B	5	0	0	0	0
4	A	411	0	0	43	0
4	B	399	0	0	55	2
All	All	9763	0	8664	227	2

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 13.

All (227) 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:A:474:LYS:NZ	4:A:992:HOH:O	1.87	1.05
1:B:59:GLN:O	4:B:907:HOH:O	1.81	0.95
1:A:505:GLU:OE1	4:A:803:HOH:O	1.83	0.94
1:B:94:ASP:OD1	4:B:899:HOH:O	1.84	0.93
1:B:234:MET:O	4:B:835:HOH:O	1.87	0.93
1:A:425:GLU:OE1	4:A:1079:HOH:O	1.86	0.92
1:B:88:ASN:ND2	4:B:1015:HOH:O	2.10	0.83
1:A:302:THR:O	4:A:842:HOH:O	1.95	0.81
2:B:602:MPO:O1	4:B:842:HOH:O	1.97	0.81
1:A:118:GLN:OE1	4:A:894:HOH:O	1.99	0.80
1:B:107:TYR:O	4:B:822:HOH:O	1.99	0.80
1:B:294:ARG:NH1	4:B:980:HOH:O	2.15	0.80
1:A:112:SER:O	4:A:701:HOH:O	2.00	0.79
1:B:292:SER:OG	4:B:972:HOH:O	2.01	0.79
1:B:159:ILE:N	4:B:704:HOH:O	2.15	0.79
1:B:275:ASP:OD2	4:B:1053:HOH:O	2.02	0.78
1:A:265:ARG:HG2	1:A:265:ARG:HH11	1.47	0.76
1:B:359:SER:OG	4:B:782:HOH:O	2.03	0.75
1:A:555:ASN:OD1	4:A:810:HOH:O	2.05	0.74
1:B:447:THR:OG1	4:B:791:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:GLN:NE2	4:B:707:HOH:O	2.20	0.73
1:B:243:LEU:O	4:B:701:HOH:O	2.07	0.73
1:B:139:THR:OG1	4:B:822:HOH:O	2.08	0.72
1:B:505:GLU:OE1	4:B:826:HOH:O	2.06	0.72
1:A:34:HIS:NE2	4:A:1010:HOH:O	2.22	0.71
1:B:522:LEU:O	1:B:555:ASN:ND2	2.23	0.71
1:A:265:ARG:NH1	1:A:283:ARG:HA	2.06	0.71
1:A:127:GLY:O	4:A:1027:HOH:O	2.09	0.71
1:A:200:ASP:OD1	4:A:702:HOH:O	2.08	0.70
1:A:284:ASP:OD2	4:A:786:HOH:O	2.11	0.69
1:A:405:LEU:O	4:A:1004:HOH:O	2.11	0.69
1:B:571:LYS:NZ	4:B:955:HOH:O	2.27	0.68
1:B:101:SER:OG	4:B:702:HOH:O	2.11	0.68
1:A:112:SER:OG	4:A:794:HOH:O	2.11	0.68
1:A:359:SER:OG	4:A:1072:HOH:O	2.11	0.68
1:A:50:GLY:O	4:A:1078:HOH:O	2.12	0.67
1:A:321:VAL:O	4:A:1019:HOH:O	2.12	0.67
1:A:208:TYR:HB3	1:A:210:MET:HE3	1.75	0.66
1:B:247:PHE:O	4:B:703:HOH:O	2.13	0.66
1:B:54:SER:O	4:B:886:HOH:O	2.13	0.66
1:B:555:ASN:OD1	4:B:901:HOH:O	2.14	0.65
1:B:406:LEU:O	4:B:827:HOH:O	2.14	0.65
1:B:399:LYS:O	4:B:969:HOH:O	2.15	0.65
1:B:184:GLY:O	4:B:836:HOH:O	2.14	0.65
1:A:172:ASP:O	4:A:703:HOH:O	2.13	0.64
1:A:48:GLU:O	4:A:921:HOH:O	2.15	0.64
1:B:84:GLU:OE1	4:B:817:HOH:O	2.14	0.64
1:A:117:GLN:N	4:A:896:HOH:O	2.30	0.64
1:A:249:ASP:OD2	4:A:877:HOH:O	2.15	0.64
1:A:116:LEU:HB3	4:A:896:HOH:O	1.98	0.64
1:A:316:LEU:O	1:A:334:ALA:N	2.30	0.63
1:B:145:SER:HB3	1:B:170:PRO:HB3	1.81	0.63
1:A:265:ARG:HG2	1:A:265:ARG:NH1	2.13	0.63
1:B:137:THR:HG23	1:B:176:PHE:HB3	1.81	0.62
1:B:8:PRO:HB3	1:B:12:LEU:O	1.98	0.62
1:B:120:LYS:NZ	4:B:968:HOH:O	2.33	0.62
1:A:389:TRP:NE1	1:A:477:GLU:OE2	2.31	0.61
1:B:4:LYS:O	4:B:705:HOH:O	2.16	0.61
1:A:171:PHE:CE1	2:A:601:MPO:H42	2.36	0.61
1:B:500:ILE:HB	2:B:602:MPO:H11	1.83	0.60
1:A:503:ILE:HD12	1:A:504:ILE:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TYR:OH	4:A:896:HOH:O	2.04	0.59
1:B:500:ILE:HD12	2:B:602:MPO:H52	1.83	0.59
1:B:386[A]:GLN:NE2	4:B:1027:HOH:O	2.34	0.59
1:A:323:VAL:O	4:A:1087:HOH:O	2.17	0.59
1:A:522:LEU:O	1:A:555:ASN:ND2	2.26	0.58
1:A:500:ILE:HB	2:A:601:MPO:H22	1.85	0.58
1:B:503:ILE:HG23	1:B:516:PHE:HB3	1.86	0.58
1:A:425:GLU:O	4:A:1090:HOH:O	2.17	0.57
1:B:358:ASN:OD1	1:B:372:SER:OG	2.21	0.57
1:B:556:GLN:HG2	4:B:803:HOH:O	2.05	0.57
1:B:380:LYS:NZ	1:B:477:GLU:OE2	2.26	0.57
1:B:253:GLU:HG3	1:B:254:SER:N	2.19	0.57
1:B:428:ASP:O	4:B:898:HOH:O	2.17	0.57
1:A:317:ASP:OD1	1:A:319:GLY:N	2.37	0.56
1:B:1:ALA:O	4:B:706:HOH:O	2.18	0.56
1:B:131:ARG:NH2	1:B:510:ARG:HD2	2.20	0.56
1:B:203:ILE:O	4:B:801:HOH:O	2.18	0.56
1:A:208:TYR:O	1:A:210:MET:HG3	2.06	0.56
1:A:171:PHE:CE2	1:A:210:MET:HE1	2.40	0.56
1:B:265:ARG:CZ	1:B:283:ARG:HG2	2.36	0.56
1:A:380:LYS:HG2	1:A:388:LYS:HB2	1.88	0.56
1:B:284:ASP:O	1:B:285:HIS:ND1	2.39	0.56
1:A:275:ASP:OD2	4:A:882:HOH:O	2.18	0.56
1:B:62:LEU:N	4:B:907:HOH:O	2.38	0.55
1:A:355:ALA:O	1:A:373:SER:OG	2.20	0.55
1:B:395:LYS:NZ	4:B:854:HOH:O	2.39	0.55
1:A:136:ASN:ND2	4:A:796:HOH:O	2.30	0.54
1:A:410:ASP:OD1	1:A:413:GLY:N	2.40	0.54
1:A:487:GLU:O	1:A:541:LYS:HE3	2.07	0.54
1:B:300:ASP:O	1:B:304:ILE:HG13	2.08	0.54
1:B:62:LEU:O	1:B:66:ASP:N	2.41	0.54
1:B:501:THR:N	2:B:602:MPO:O3	2.40	0.54
1:A:171:PHE:HE1	2:A:601:MPO:H42	1.73	0.54
1:B:143:GLN:NE2	4:B:1037:HOH:O	2.40	0.54
1:A:145:SER:HB3	1:A:170:PRO:HB3	1.90	0.54
1:B:251:THR:OG1	1:B:265:ARG:NH1	2.39	0.53
1:B:386[B]:GLN:NE2	4:B:1027:HOH:O	2.40	0.53
1:B:388:LYS:NZ	4:B:1023:HOH:O	2.42	0.53
1:A:566:PRO:HA	1:A:569:MET:HG3	1.91	0.53
1:B:308:LYS:NZ	4:B:881:HOH:O	2.42	0.53
1:B:356:HIS:HB3	1:B:374:ARG:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:LYS:O	4:B:926:HOH:O	2.18	0.53
1:B:154:ASP:OD1	1:B:157:ALA:HB2	2.09	0.53
1:A:85:TRP:HB2	4:A:908:HOH:O	2.10	0.52
1:A:136:ASN:OD1	4:A:1040:HOH:O	2.19	0.52
1:A:423:LEU:HA	1:A:456:HIS:CE1	2.44	0.52
1:A:24:PRO:O	4:A:705:HOH:O	2.19	0.52
1:A:200:ASP:CG	4:A:702:HOH:O	2.53	0.52
1:A:490:LYS:HB2	4:A:823:HOH:O	2.09	0.51
1:B:48:GLU:OE1	1:B:48:GLU:N	2.42	0.51
1:B:443:LYS:NZ	4:B:944:HOH:O	1.92	0.51
1:B:319:GLY:HA3	1:B:330:ALA:HA	1.92	0.51
1:B:63:LYS:N	4:B:907:HOH:O	2.01	0.51
1:B:358:ASN:ND2	2:B:602:MPO:O2	2.35	0.51
1:A:160:LEU:O	4:A:704:HOH:O	2.19	0.51
1:A:122:ILE:HB	1:A:546:GLU:O	2.11	0.51
1:B:284:ASP:OD2	4:B:929:HOH:O	2.19	0.51
1:A:294:ARG:NH1	1:B:60:GLU:OE1	2.42	0.50
1:A:427:SER:OG	4:A:999:HOH:O	2.19	0.50
1:B:419:ASN:O	4:B:975:HOH:O	2.19	0.50
1:A:245:ARG:HD3	1:B:65:TYR:O	2.11	0.50
1:B:34:HIS:NE2	4:B:833:HOH:O	2.34	0.50
1:A:28:LEU:HD12	1:A:68:VAL:O	2.11	0.50
1:A:290:ASP:HB2	4:A:819:HOH:O	2.11	0.50
1:B:250:ALA:HB2	1:B:266:VAL:HG12	1.93	0.50
1:A:8:PRO:HB3	1:A:12:LEU:O	2.12	0.49
1:A:400:PRO:O	1:A:403:SER:OG	2.29	0.49
1:A:366:ASP:OD1	1:A:368:SER:OG	2.23	0.49
1:A:48:GLU:H	1:A:48:GLU:CD	2.20	0.49
1:A:188:TRP:CH2	1:A:190:LEU:HB2	2.47	0.49
1:A:503:ILE:HG23	1:A:516:PHE:HB3	1.94	0.49
1:B:390:ILE:HB	1:B:405:LEU:HD23	1.94	0.49
1:A:374:ARG:HD3	1:A:375:HIS:CD2	2.48	0.48
1:A:390:ILE:HB	1:A:405:LEU:HD23	1.95	0.48
1:B:553:LYS:NZ	4:B:822:HOH:O	2.47	0.48
1:A:272:ARG:NH1	4:A:969:HOH:O	2.44	0.48
1:B:188:TRP:CH2	1:B:190:LEU:HB2	2.49	0.48
1:B:368:SER:OG	1:B:380:LYS:HE2	2.14	0.48
1:A:361:ALA:HB3	1:A:370:ILE:HB	1.96	0.47
1:A:418:CYS:HA	1:A:424:CYS:HA	1.96	0.47
1:A:265:ARG:HH12	1:A:283:ARG:HA	1.76	0.47
1:A:286:ILE:HB	1:A:299:TRP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ALA:HB1	4:B:941:HOH:O	2.14	0.47
1:A:123:LYS:HD2	4:A:880:HOH:O	2.14	0.47
1:B:385:LYS:NZ	4:B:999:HOH:O	2.47	0.47
1:B:307:PRO:HA	1:B:354:TRP:CE3	2.50	0.47
1:B:148:HIS:HD2	4:B:808:HOH:O	1.98	0.47
1:A:265:ARG:HH11	1:A:265:ARG:CG	2.14	0.46
1:B:353:ASN:ND2	4:B:855:HOH:O	2.08	0.46
1:B:128:PHE:O	1:B:182:THR:HG21	2.15	0.46
1:A:58:GLY:HA3	1:A:571:LYS:O	2.14	0.46
1:A:422:GLY:HA3	1:A:433:TYR:OH	2.15	0.46
1:A:501:THR:HG22	2:A:601:MPO:H21	1.96	0.46
1:B:310:ASP:HA	1:B:313:LEU:HD12	1.97	0.46
1:A:383:ARG:O	1:A:385:LYS:NZ	2.48	0.46
1:B:421:ASN:ND2	4:B:964:HOH:O	2.49	0.46
1:B:438:ALA:HB1	1:B:446:LEU:HD11	1.98	0.46
1:B:268:LYS:HB2	1:B:285:HIS:CD2	2.51	0.46
1:A:300:ASP:O	1:A:304:ILE:HG13	2.16	0.45
1:B:379:VAL:HG12	1:B:390:ILE:HG12	1.98	0.45
1:A:209:LEU:N	4:A:1005:HOH:O	2.33	0.45
1:A:433:TYR:O	1:A:434:THR:OG1	2.30	0.45
1:B:503:ILE:HD12	1:B:504:ILE:N	2.31	0.45
1:B:566:PRO:HA	1:B:569:MET:HG3	1.98	0.45
1:A:131:ARG:NH2	1:A:510:ARG:HD2	2.32	0.45
1:B:433:TYR:O	1:B:434:THR:OG1	2.33	0.45
1:A:251:THR:OG1	1:A:265:ARG:NH2	2.46	0.44
1:B:60:GLU:HG3	4:B:1055:HOH:O	2.17	0.44
1:B:409:VAL:HG12	1:B:415:PRO:HA	1.99	0.44
1:A:208:TYR:CD1	1:A:210:MET:HE2	2.52	0.44
1:B:507:GLN:HE21	1:B:514:PHE:HB3	1.82	0.44
1:B:85:TRP:CE2	1:B:92:MET:HB2	2.52	0.44
1:A:48:GLU:CD	1:A:48:GLU:N	2.75	0.44
1:A:153:LYS:NZ	1:A:161:ASP:O	2.42	0.44
1:A:171:PHE:CD2	1:A:251:THR:HG21	2.52	0.44
1:B:417:THR:O	1:B:425:GLU:HG2	2.17	0.44
1:A:131:ARG:HD2	1:A:563:LEU:HD21	1.99	0.44
1:B:137:THR:OG1	1:B:138:HIS:N	2.51	0.44
1:A:470:PHE:O	1:A:487:GLU:HA	2.18	0.44
1:B:553:LYS:HB2	1:B:556:GLN:OE1	2.18	0.44
1:A:80:LYS:NZ	4:A:1017:HOH:O	2.29	0.43
1:A:340:THR:O	1:A:352:ARG:NE	2.43	0.43
2:A:601:MPO:H21	2:A:601:MPO:H72	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:THR:O	1:A:437:THR:OG1	2.30	0.43
1:B:383:ARG:O	1:B:385:LYS:NZ	2.51	0.43
1:A:307:PRO:HA	1:A:354:TRP:CE3	2.54	0.43
1:B:57:VAL:HG11	1:B:69:PRO:HD2	2.01	0.43
1:A:15:VAL:HG22	1:A:29:VAL:HG22	2.00	0.43
1:B:359:SER:C	4:B:782:HOH:O	2.62	0.43
1:A:65:TYR:O	1:B:245:ARG:HD3	2.19	0.42
1:A:271:TYR:O	1:A:278:HIS:HA	2.19	0.42
1:B:467:TYR:CD2	1:B:490:LYS:HA	2.53	0.42
1:B:179:ILE:HG13	1:B:188:TRP:HB3	2.01	0.42
1:B:28:LEU:HD12	1:B:68:VAL:O	2.20	0.42
1:B:31:LEU:HD12	1:B:31:LEU:HA	1.81	0.42
1:B:312:LEU:HA	1:B:457:LEU:HD22	2.02	0.42
1:A:11:GLN:HG3	1:A:94:ASP:OD1	2.20	0.42
1:A:40:LYS:HE2	1:A:40:LYS:HB3	1.65	0.42
1:A:265:ARG:HB2	1:A:360:ILE:HD11	2.01	0.42
1:A:492:ARG:HE	1:A:492:ARG:HB3	1.67	0.42
1:A:359:SER:HB2	1:A:437:THR:HA	2.02	0.41
1:B:92:MET:HE3	1:B:92:MET:HB3	1.80	0.41
1:A:210:MET:SD	1:A:252:HIS:N	2.83	0.41
1:A:308:LYS:NZ	4:A:1046:HOH:O	2.53	0.41
1:B:29:VAL:HB	1:B:68:VAL:HB	2.02	0.41
1:A:27:ALA:HB3	1:A:70:ILE:HB	2.01	0.41
1:A:442:SER:OG	4:A:964:HOH:O	2.21	0.41
1:B:24:PRO:HD2	1:B:189:TRP:O	2.20	0.41
1:B:309:ARG:O	1:B:313:LEU:HD12	2.20	0.41
1:B:420:GLU:HG3	1:B:421:ASN:OD1	2.21	0.41
1:B:477:GLU:OE2	4:B:923:HOH:O	2.22	0.41
1:A:230:GLU:HB3	1:A:239:GLU:HG3	2.03	0.41
1:A:392:ALA:HB1	4:A:989:HOH:O	2.20	0.41
1:A:265:ARG:CZ	1:A:283:ARG:HG2	2.50	0.41
1:B:560:ARG:HD2	4:B:875:HOH:O	2.21	0.41
1:A:509:ASP:OD1	1:A:510:ARG:N	2.54	0.41
1:B:60:GLU:C	4:B:907:HOH:O	2.64	0.41
1:A:456:HIS:CE1	4:A:1013:HOH:O	2.73	0.40
1:B:28:LEU:HD12	1:B:68:VAL:C	2.45	0.40
1:B:339:ASP:OD1	1:B:339:ASP:N	2.51	0.40
1:A:29:VAL:HG23	1:A:70:ILE:HD11	2.03	0.40
1:A:137:THR:OG1	1:A:138:HIS:N	2.54	0.40
1:A:299:TRP:CD1	1:A:385:LYS:HD3	2.56	0.40
1:A:435:GLN:CD	1:A:435:GLN:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:TYR:OH	4:A:909:HOH:O	2.06	0.40
1:B:498:SER:HA	1:B:499:PRO:HD2	1.89	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	Interatomic distance (Å)	Clash overlap (Å)
4:B:765:HOH:O	4:B:770:HOH:O[4_667]	1.83	0.37
1:B:115:ASP:OD2	4:B:702:HOH:O[4_667]	2.19	0.01

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	565/571 (99%)	524 (93%)	38 (7%)	3 (0%)	24	16
1	B	562/571 (98%)	524 (93%)	36 (6%)	2 (0%)	30	21
All	All	1127/1142 (99%)	1048 (93%)	74 (7%)	5 (0%)	30	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	VAL
1	A	437	THR
1	B	311	ALA
1	B	524	ASP
1	A	501	THR

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	474/483 (98%)	465 (98%)	9 (2%)	50	45
1	B	472/483 (98%)	466 (99%)	6 (1%)	61	58
All	All	946/966 (98%)	931 (98%)	15 (2%)	55	52

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	LYS
1	A	121	VAL
1	A	159	ILE
1	A	298	VAL
1	A	359	SER
1	A	427	SER
1	A	475	ILE
1	A	503	ILE
1	A	547	ILE
1	B	49	LYS
1	B	148	HIS
1	B	265	ARG
1	B	304	ILE
1	B	372	SER
1	B	503	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	224	GLN
1	A	270	ASN
1	A	329	HIS
1	A	332	GLN
1	A	353	ASN
1	A	375	HIS
1	A	412	ASN
1	A	456	HIS
1	B	11	GLN
1	B	22	ASN

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Mol	Chain	Res	Type
1	B	106	ASN
1	B	148	HIS
1	B	236	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	601	-	4,4,4	0.22	0	6,6,6	0.10	0
2	MPO	B	602	-	13,13,13	1.82	4 (30%)	17,17,17	2.21	5 (29%)
2	MPO	A	601	-	13,13,13	1.66	4 (30%)	17,17,17	2.47	6 (35%)

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
2	MPO	B	602	-	-	4/7/15/15	0/1/1/1
2	MPO	A	601	-	-	1/7/15/15	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	MPO	C1-S1	4.28	1.83	1.77
2	A	601	MPO	C1-S1	3.42	1.82	1.77
2	B	602	MPO	O1-S1	2.75	1.52	1.45
2	A	601	MPO	O1-S1	2.50	1.52	1.45
2	A	601	MPO	O3-S1	2.33	1.55	1.47
2	B	602	MPO	C3-N1	-2.33	1.42	1.47
2	B	602	MPO	O3-S1	2.30	1.55	1.47
2	A	601	MPO	C3-N1	-2.15	1.42	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	MPO	C2-C1-S1	-6.05	103.97	113.25
2	B	602	MPO	O3-S1-O2	-4.89	99.15	111.40
2	B	602	MPO	O3-S1-C1	4.41	114.63	106.00
2	A	601	MPO	C2-C3-N1	-4.15	102.27	113.93
2	A	601	MPO	O3-S1-O2	-3.94	101.53	111.40
2	A	601	MPO	O2-S1-C1	3.82	112.51	106.73
2	B	602	MPO	C7-N1-C4	3.55	116.48	108.84
2	A	601	MPO	C7-N1-C4	3.04	115.38	108.84
2	B	602	MPO	C5-C4-N1	2.70	114.23	110.12
2	B	602	MPO	C6-C7-N1	2.04	113.22	110.12
2	A	601	MPO	C5-C4-N1	2.02	113.19	110.12

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	602	MPO	S1-C1-C2-C3
2	B	602	MPO	C1-C2-C3-N1
2	B	602	MPO	C2-C1-S1-O1
2	A	601	MPO	C1-C2-C3-N1
2	B	602	MPO	C2-C3-N1-C7

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	MPO	5	0
2	A	601	MPO	5	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	567/571 (99%)	-1.32	0 100 100	31, 40, 62, 95	2 (0%)
1	B	563/571 (98%)	-1.31	0 100 100	30, 41, 67, 115	3 (0%)
All	All	1130/1142 (98%)	-1.31	0 100 100	30, 41, 65, 115	5 (0%)

There are no RSRZ outliers to report.

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
2	MPO	B	602	13/13	0.97	0.07	40,46,56,58	0
2	MPO	A	601	13/13	0.99	0.06	41,54,69,75	0
3	SO4	B	601	5/5	0.99	0.03	54,57,60,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.