Full wwPDB X-ray Structure Validation Report

Jan 30, 2021 – 03:04 PM EST

PDB ID	:	3ED4
Title	:	Crystal structure of putative arylsulfatase from escherichia coli
Authors	:	Patskovsky, Y.; Ozyurt, S.; Gilmore, M.; Chang, S.; Bain, K.; Wasserman, S.; Koss, J.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-09-02
Resolution	:	1.70 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 following versions of software and data (see references ⓘ) were used in the production of this report:

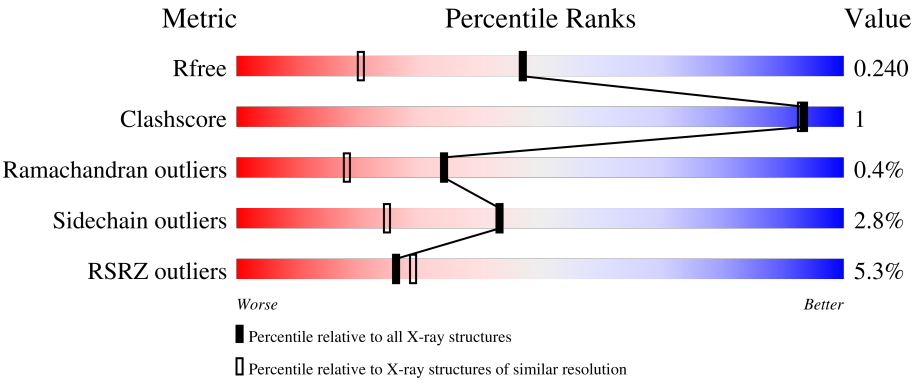
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	502	4% 88% 5% 7%
1	B	502	2% 90% · 6%
1	C	502	8% 88% · 7%
1	D	502	6% 87% 7% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	1	-	-	X	-
5	UNL	D	520	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16828 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 ARYLSULFATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	12	0
			3800	2426	642	714	18			
1	B	474	Total	C	N	O	S	0	7	0
			3807	2428	643	718	18			
1	C	467	Total	C	N	O	S	0	4	0
			3747	2390	633	706	18			
1	D	474	Total	C	N	O	S	0	18	0
			3883	2481	658	725	19			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP Q8FLC3
A	17	SER	-	expression tag	UNP Q8FLC3
A	18	LEU	-	expression tag	UNP Q8FLC3
A	510	GLU	-	expression tag	UNP Q8FLC3
A	511	GLY	-	expression tag	UNP Q8FLC3
A	512	HIS	-	expression tag	UNP Q8FLC3
A	513	HIS	-	expression tag	UNP Q8FLC3
A	514	HIS	-	expression tag	UNP Q8FLC3
A	515	HIS	-	expression tag	UNP Q8FLC3
A	516	HIS	-	expression tag	UNP Q8FLC3
A	517	HIS	-	expression tag	UNP Q8FLC3
B	16	MET	-	expression tag	UNP Q8FLC3
B	17	SER	-	expression tag	UNP Q8FLC3
B	18	LEU	-	expression tag	UNP Q8FLC3
B	510	GLU	-	expression tag	UNP Q8FLC3
B	511	GLY	-	expression tag	UNP Q8FLC3
B	512	HIS	-	expression tag	UNP Q8FLC3
B	513	HIS	-	expression tag	UNP Q8FLC3
B	514	HIS	-	expression tag	UNP Q8FLC3
B	515	HIS	-	expression tag	UNP Q8FLC3
B	516	HIS	-	expression tag	UNP Q8FLC3

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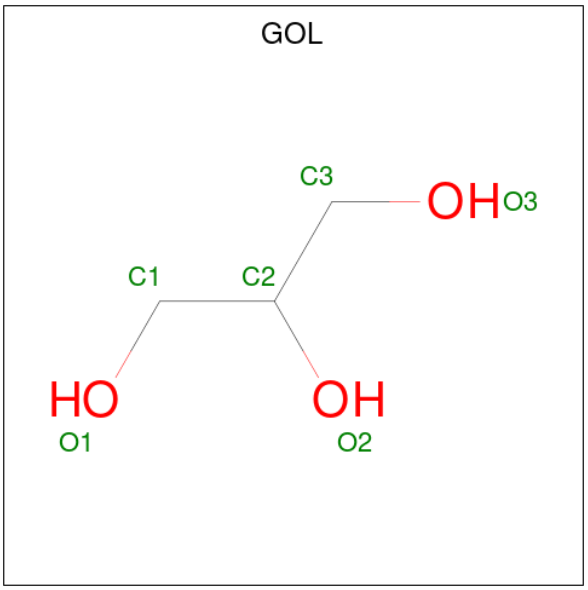
Chain	Residue	Modelled	Actual	Comment	Reference
B	517	HIS	-	expression tag	UNP Q8FLC3
C	16	MET	-	expression tag	UNP Q8FLC3
C	17	SER	-	expression tag	UNP Q8FLC3
C	18	LEU	-	expression tag	UNP Q8FLC3
C	510	GLU	-	expression tag	UNP Q8FLC3
C	511	GLY	-	expression tag	UNP Q8FLC3
C	512	HIS	-	expression tag	UNP Q8FLC3
C	513	HIS	-	expression tag	UNP Q8FLC3
C	514	HIS	-	expression tag	UNP Q8FLC3
C	515	HIS	-	expression tag	UNP Q8FLC3
C	516	HIS	-	expression tag	UNP Q8FLC3
C	517	HIS	-	expression tag	UNP Q8FLC3
D	16	MET	-	expression tag	UNP Q8FLC3
D	17	SER	-	expression tag	UNP Q8FLC3
D	18	LEU	-	expression tag	UNP Q8FLC3
D	510	GLU	-	expression tag	UNP Q8FLC3
D	511	GLY	-	expression tag	UNP Q8FLC3
D	512	HIS	-	expression tag	UNP Q8FLC3
D	513	HIS	-	expression tag	UNP Q8FLC3
D	514	HIS	-	expression tag	UNP Q8FLC3
D	515	HIS	-	expression tag	UNP Q8FLC3
D	516	HIS	-	expression tag	UNP Q8FLC3
D	517	HIS	-	expression tag	UNP Q8FLC3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

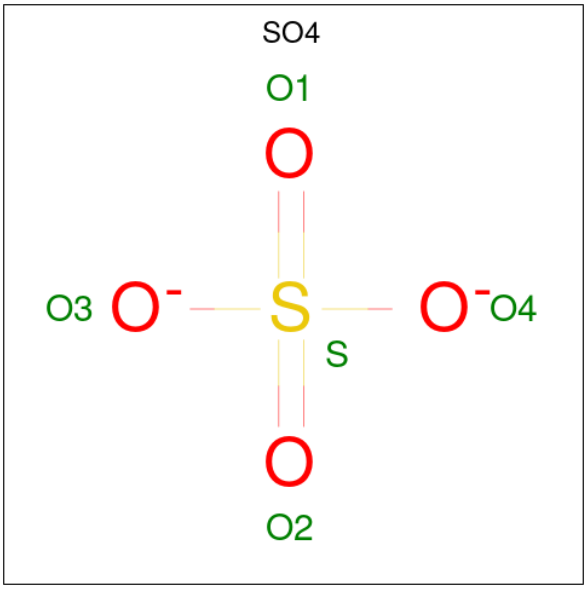


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	2	Total Na 2 2	0	0
3	D	1	Total Na 1 1	0	0
3	C	2	Total Na 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 1 3	0	0
5	A	1	Total C O 4 1 3	0	0
5	D	3	Total C O 12 3 9	0	0
5	C	1	Total C O 4 1 3	0	0

- Molecule 6 is water.

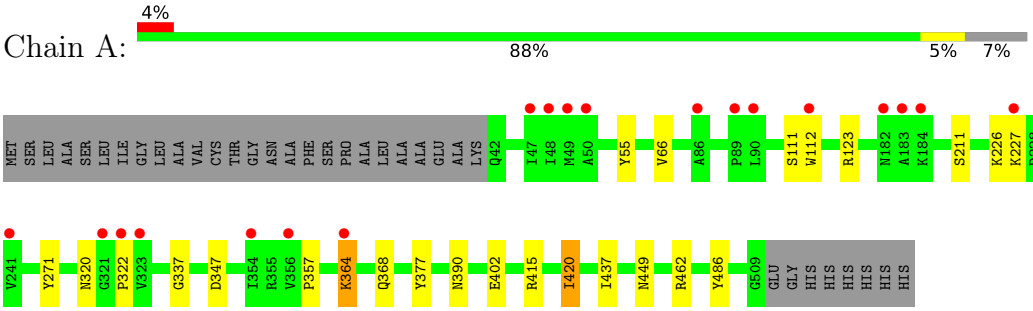
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	387	Total O 387 387	0	0
6	B	438	Total O 438 438	0	0
6	C	315	Total O 315 315	0	0
6	D	382	Total O 383 383	0	1

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.

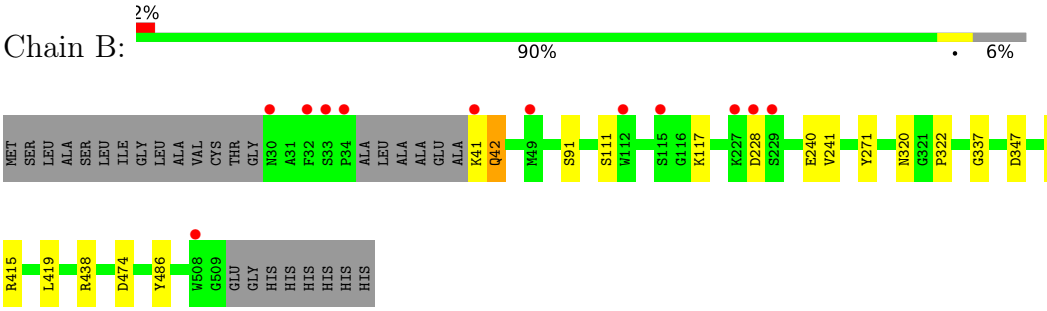
• Molecule 1: ARYLSULFATASE

Chain A:



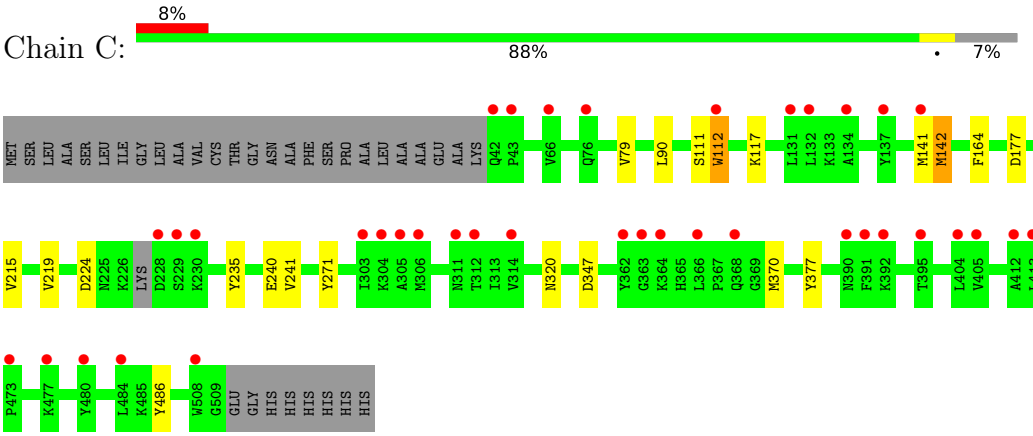
• Molecule 1: ARYLSULFATASE

Chain B:



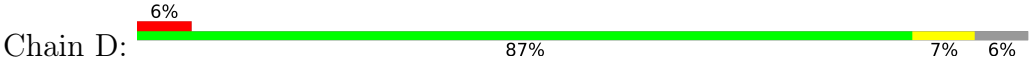
• Molecule 1: ARYLSULFATASE

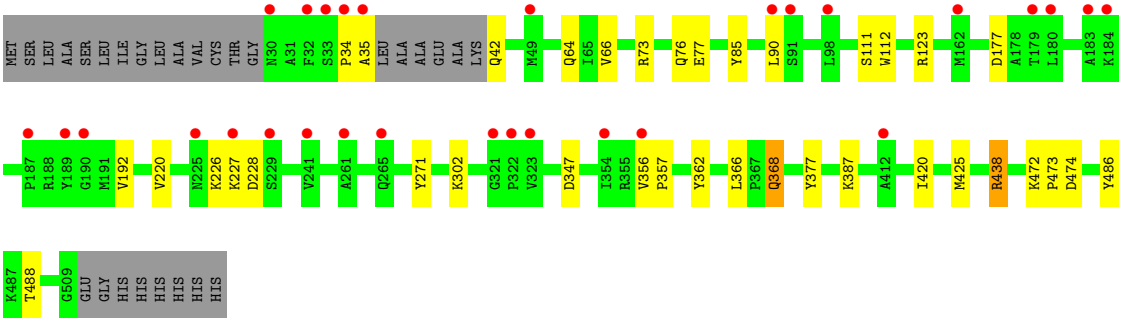
Chain C:



• Molecule 1: ARYLSULFATASE

Chain D:




MET SER LEU ALA SER LEU ILE GLY LEU ALA VAL CYS THR GLY N30 A31 F32 S33 P34 A35 LEU ALA ALA GLU ALA LYS Q42 M49 Q64 I65 V66 R73 Q76 E77 Y85 L90 S91 L98 S111 W112 R123 M162 D177 A178 T179 L180 A183 K184
P187 R188 Y189 G190 M191 V192 V220 N225 K226 K227 D228 S229 V241 A261 Q265 Y271 K302 G321 P322 V323 D347 I354 R355 V356 P357 Y362 L366 P367 Q368 Y377 K387 A412 I420 M425 R438 K472 P473 D474 Y486
K487 T488 G509 GLU GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.93Å 178.86Å 76.28Å 90.00° 92.17° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 39.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	87.3 (20.00-1.70) 87.2 (39.74-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.196 , 0.242 0.194 , 0.240	Depositor DCC
R_{free} test set	5541 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16828	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: GOL, UNL, SO4, NA

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	0.49	0/3921	0.60	0/5308
1	B	0.48	0/3923	0.60	0/5312
1	C	0.43	0/3851	0.59	1/5216 (0.0%)
1	D	0.47	0/4032	0.64	1/5455 (0.0%)
All	All	0.47	0/15727	0.61	2/21291 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	90	LEU	CA-CB-CG	5.49	127.93	115.30
1	C	90	LEU	CA-CB-CG	5.06	126.94	115.30

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	3800	0	3773	9	0
1	B	3807	0	3760	11	0
1	C	3747	0	3683	9	0
1	D	3883	0	3876	14	0
2	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	14	6	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	12	0	0	4	0
6	A	387	0	0	1	0
6	B	438	0	0	0	0
6	C	315	0	0	0	0
6	D	383	0	0	1	0
All	All	16828	0	15114	43	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 1.

All (43) 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:462:ARG:HH21	2:A:1:GOL:H32	1.34	0.88
1:A:239[B]:THR:HG23	6:A:802:HOH:O	1.93	0.67
1:B:375:PRO:HB2	2:B:1:GOL:H31	1.77	0.66
1:B:375:PRO:CB	2:B:1:GOL:H31	2.29	0.63
1:D:34:PRO:HA	1:D:35:ALA:HB3	1.82	0.62
1:D:473:PRO:HD2	5:D:520:UNL:O2	2.01	0.60
1:B:375:PRO:HG2	2:B:1:GOL:H31	1.83	0.58
1:A:420:ILE:HD12	1:A:437[A]:ILE:HG22	1.85	0.58
1:A:462:ARG:NH2	2:A:1:GOL:H32	2.13	0.56
1:B:438:ARG:HG3	2:B:1:GOL:O2	2.06	0.55
1:D:123[A]:ARG:HG3	1:D:123[A]:ARG:HH21	1.72	0.54
1:D:64:GLN:NE2	5:D:518:UNL:O2	2.40	0.54
1:B:375:PRO:CG	2:B:1:GOL:H31	2.39	0.53
1:C:112[A]:TRP:CZ2	1:C:425:MET:HG3	2.44	0.52
1:C:141:MET:HB2	1:C:164:PHE:CD1	2.44	0.52
1:D:474:ASP:HB2	5:D:520:UNL:O3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:SER:OG	4:B:2:SO4:O1	2.31	0.49
1:D:77:GLU:HA	1:D:368:GLN:HG3	1.95	0.48
1:A:55:TYR:HA	1:A:357:PRO:HD3	1.96	0.48
1:C:141:MET:HG3	1:C:235:TYR:HD2	1.79	0.47
1:B:419:LEU:HB2	1:B:438:ARG:HB3	1.95	0.47
1:A:402:GLU:HG3	1:A:415:ARG:HG3	1.97	0.47
1:A:364:LYS:HA	1:A:368:GLN:HE22	1.80	0.47
1:C:215:VAL:O	1:C:219:VAL:HG23	2.15	0.47
1:D:112:TRP:CZ2	1:D:425:MET:HG3	2.51	0.46
1:D:220:VAL:HG13	1:D:302:LYS:HD3	1.98	0.45
1:A:211:SER:OG	1:A:239[B]:THR:HG21	2.16	0.45
1:D:356:VAL:HB	1:D:357:PRO:HD2	1.98	0.45
1:D:76[A]:GLN:NE2	6:D:618:HOH:O	2.50	0.44
1:B:240:GLU:HA	1:B:241:VAL:HA	1.84	0.44
1:C:142:MET:HB2	1:C:142:MET:HE2	1.73	0.43
1:C:79:VAL:HG22	1:C:370:MET:HB3	2.00	0.43
1:D:177:ASP:HB2	1:D:192:VAL:HG13	1.99	0.43
1:D:85:TYR:OH	1:D:438[B]:ARG:NH1	2.51	0.43
1:A:322:PRO:HB2	1:A:337:GLY:HA3	2.01	0.42
1:C:240:GLU:HA	1:C:241:VAL:HA	1.82	0.41
1:C:414:LYS:HA	1:C:414:LYS:HD2	1.86	0.41
1:C:177:ASP:HB2	1:C:192:VAL:HG13	2.02	0.41
1:B:415:ARG:HG3	2:B:1:GOL:H11	2.01	0.41
1:D:472:LYS:HD3	5:D:520:UNL:O1	2.20	0.41
1:B:42:GLN:H	1:B:42:GLN:HG2	1.59	0.41
1:B:322:PRO:HB2	1:B:337:GLY:HA3	2.02	0.40
1:D:362:TYR:HB3	1:D:366:LEU:HG	2.04	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	478/502 (95%)	462 (97%)	14 (3%)	2 (0%)	34	18
1	B	477/502 (95%)	465 (98%)	10 (2%)	2 (0%)	34	18
1	C	467/502 (93%)	447 (96%)	18 (4%)	2 (0%)	34	18
1	D	489/502 (97%)	476 (97%)	11 (2%)	2 (0%)	34	18
All	All	1911/2008 (95%)	1850 (97%)	53 (3%)	8 (0%)	34	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	ASP
1	C	347	ASP
1	D	111	SER
1	D	347	ASP
1	A	111	SER
1	B	111	SER
1	B	347	ASP
1	C	111	SER

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	408/420 (97%)	394 (97%)	14 (3%)	37	18
1	B	408/420 (97%)	398 (98%)	10 (2%)	47	29
1	C	399/420 (95%)	389 (98%)	10 (2%)	47	29
1	D	419/420 (100%)	404 (96%)	15 (4%)	35	16
All	All	1634/1680 (97%)	1585 (97%)	49 (3%)	43	22

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	112	TRP
1	A	123	ARG

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Mol	Chain	Res	Type
1	A	226[A]	LYS
1	A	226[B]	LYS
1	A	227	LYS
1	A	271	TYR
1	A	320	ASN
1	A	364	LYS
1	A	377	TYR
1	A	390	ASN
1	A	420	ILE
1	A	449	ASN
1	A	486	TYR
1	B	41	LYS
1	B	42	GLN
1	B	117	LYS
1	B	228	ASP
1	B	271	TYR
1	B	320	ASN
1	B	377	TYR
1	B	474[A]	ASP
1	B	474[B]	ASP
1	B	486	TYR
1	C	112[A]	TRP
1	C	112[B]	TRP
1	C	117[A]	LYS
1	C	117[B]	LYS
1	C	142	MET
1	C	224	ASP
1	C	271	TYR
1	C	320	ASN
1	C	377	TYR
1	C	486	TYR
1	D	42	GLN
1	D	66	VAL
1	D	73	ARG
1	D	226	LYS
1	D	227	LYS
1	D	228	ASP
1	D	271	TYR
1	D	368	GLN
1	D	377	TYR
1	D	387	LYS
1	D	420	ILE

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Mol	Chain	Res	Type
1	D	438[A]	ARG
1	D	438[B]	ARG
1	D	486	TYR
1	D	488	THR

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	295	GLN
1	A	368	GLN
1	B	30	ASN
1	B	42	GLN
1	B	64	GLN
1	B	225	ASN
1	B	449	ASN
1	C	64	GLN
1	C	135	GLN
1	C	295	GLN
1	D	42	GLN
1	D	64	GLN
1	D	478	GLN
1	D	492	ASN

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 19 ligands modelled in this entry, 6 are unknown and 6 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
4	SO4	A	520	-	4,4,4	0.18	0	6,6,6	0.05	0
4	SO4	D	4	-	4,4,4	0.70	0	6,6,6	0.61	0
2	GOL	B	1	-	5,5,5	1.63	2 (40%)	5,5,5	0.90	0
2	GOL	A	1	-	5,5,5	0.24	0	5,5,5	0.75	0
4	SO4	C	3	-	4,4,4	0.15	0	6,6,6	0.09	0
2	GOL	B	519	-	5,5,5	0.34	0	5,5,5	0.32	0
4	SO4	B	2	-	4,4,4	0.20	0	6,6,6	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	519	-	-	4/4/4/4	-
2	GOL	B	1	-	-	2/4/4/4	-
2	GOL	A	1	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GOL	O2-C2	-2.56	1.35	1.43
2	B	1	GOL	O3-C3	-2.06	1.33	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	GOL	O2-C2-C3-O3
2	B	519	GOL	O1-C1-C2-C3
2	B	519	GOL	C1-C2-C3-O3
2	B	1	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	519	GOL	O2-C2-C3-O3
2	B	519	GOL	O1-C1-C2-O2
2	A	1	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	GOL	6	0
2	A	1	GOL	2	0
4	B	2	SO4	1	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

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	468/502 (93%)	0.21	20 (4%)	35	39	18, 30, 51, 94	0
1	B	474/502 (94%)	0.05	12 (2%)	57	61	17, 28, 51, 88	0
1	C	467/502 (93%)	0.47	39 (8%)	11	12	21, 37, 66, 87	0
1	D	474/502 (94%)	0.31	29 (6%)	21	23	19, 30, 52, 84	0
All	All	1883/2008 (93%)	0.26	100 (5%)	26	29	17, 31, 56, 94	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	35	ALA	8.9
1	C	412	ALA	6.5
1	B	34	PRO	5.5
1	C	303	ILE	5.5
1	A	227	LYS	5.2
1	D	34	PRO	5.2
1	C	405	VAL	5.1
1	C	311	ASN	4.7
1	B	229	SER	4.6
1	D	229	SER	4.6
1	B	228	ASP	4.5
1	B	30	ASN	4.5
1	C	391	PHE	4.1
1	B	33[A]	SER	4.0
1	C	229	SER	3.9
1	C	228	ASP	3.7
1	C	132	LEU	3.6
1	D	323	VAL	3.6
1	C	304	LYS	3.5
1	B	41	LYS	3.4
1	D	261	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	134	ALA	3.3
1	D	184	LYS	3.2
1	A	354	ILE	3.1
1	C	477	LYS	3.1
1	A	322	PRO	3.1
1	D	30	ASN	3.1
1	B	227	LYS	3.0
1	D	183	ALA	3.0
1	B	112	TRP	3.0
1	A	49	MET	3.0
1	D	90	LEU	3.0
1	A	183	ALA	3.0
1	C	484	LEU	2.9
1	D	49	MET	2.9
1	C	404	LEU	2.9
1	C	364	LYS	2.8
1	D	322	PRO	2.8
1	A	112	TRP	2.8
1	D	265	GLN	2.7
1	C	42	GLN	2.7
1	B	32	PHE	2.7
1	A	90	LEU	2.7
1	C	413	LEU	2.7
1	C	366	LEU	2.6
1	A	323	VAL	2.6
1	C	392	LYS	2.6
1	D	225	ASN	2.6
1	C	43	PRO	2.6
1	A	48	ILE	2.5
1	C	480	TYR	2.5
1	D	227	LYS	2.5
1	A	229	SER	2.5
1	C	305	ALA	2.5
1	D	321	GLY	2.4
1	D	187	PRO	2.4
1	C	141	MET	2.4
1	C	306	MET	2.4
1	A	364	LYS	2.4
1	D	33	SER	2.4
1	D	189	TYR	2.4
1	A	50	ALA	2.4
1	A	356	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	363	GLY	2.4
1	C	137	TYR	2.3
1	C	473	PRO	2.3
1	C	66	VAL	2.3
1	D	412	ALA	2.3
1	C	508	TRP	2.3
1	C	312	THR	2.3
1	C	395	THR	2.3
1	D	179	THR	2.3
1	B	115	SER	2.3
1	A	184	LYS	2.3
1	B	49	MET	2.3
1	A	321	GLY	2.3
1	A	241	VAL	2.3
1	C	230	LYS	2.3
1	D	162[A]	MET	2.3
1	D	190	GLY	2.3
1	C	390	ASN	2.3
1	D	180	LEU	2.2
1	D	241	VAL	2.2
1	D	354	ILE	2.2
1	B	508	TRP	2.2
1	C	362	TYR	2.1
1	C	76	GLN	2.1
1	A	89	PRO	2.1
1	C	112[A]	TRP	2.1
1	D	32	PHE	2.1
1	A	182	ASN	2.1
1	A	47	ILE	2.1
1	A	86	ALA	2.1
1	C	368	GLN	2.0
1	C	131	LEU	2.0
1	D	91	SER	2.0
1	C	189	TYR	2.0
1	C	314	VAL	2.0
1	D	356	VAL	2.0
1	D	98	LEU	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
5	UNL	A	521	4/-	0.78	0.15	30,36,44,45	0
5	UNL	C	519	4/-	0.80	0.33	34,52,57,58	0
2	GOL	B	519	6/6	0.85	0.22	48,57,62,70	0
2	GOL	B	1	6/6	0.86	0.19	24,36,59,59	0
5	UNL	D	518	4/-	0.87	0.14	31,42,50,56	0
5	UNL	D	519	4/-	0.87	0.21	52,56,58,59	0
5	UNL	B	520	4/-	0.88	0.19	25,37,44,55	0
2	GOL	A	1	6/6	0.89	0.15	24,46,52,52	0
5	UNL	D	520	4/-	0.93	0.22	54,57,61,62	0
4	SO4	D	4	5/5	0.95	0.52	25,34,47,55	5
3	NA	C	518	1/1	0.96	0.20	30,30,30,30	0
4	SO4	A	520	5/5	0.96	0.42	23,26,37,46	5
3	NA	D	1	1/1	0.97	0.25	27,27,27,27	0
4	SO4	C	3	5/5	0.98	0.20	23,31,33,50	5
3	NA	B	518	1/1	0.98	0.13	21,21,21,21	0
3	NA	C	1	1/1	0.98	0.20	19,19,19,19	0
4	SO4	B	2	5/5	0.98	0.31	24,26,40,41	5
3	NA	A	519	1/1	0.99	0.11	24,24,24,24	0
3	NA	A	518	1/1	0.99	0.18	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.