



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:18 AM GMT

PDB ID : 3LLW
Title : Crystal structure of geranyltransferase from helicobacter pylori 26695
Authors : Patskovsky, Y.; Toro, R.; Rutter, M.; Sauder, J.M.; Burley, S.K.; Almo, S.C.;
New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-01-29
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

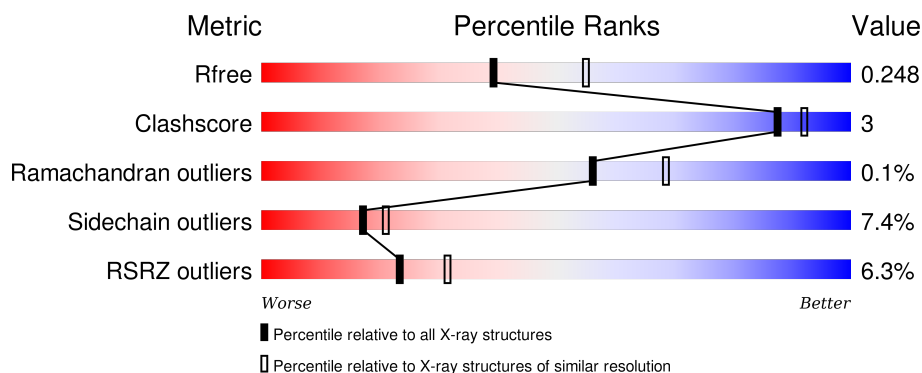
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	311	<div> <div>4%</div> <div>80%12%7%</div> </div>
1	B	311	<div> <div>7%</div> <div>84%7% • 7%</div> </div>
1	C	311	<div> <div>8%</div> <div>85%6% • 8%</div> </div>
1	D	311	<div> <div>5%</div> <div>79%13% • 7%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9399 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 Geranyltranstransferase (IspA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2298	1485	377	425	11			
1	B	288	Total	C	N	O	S	0	0	0
			2297	1484	377	425	11			
1	C	286	Total	C	N	O	S	0	0	0
			2284	1477	374	422	11			
1	D	289	Total	C	N	O	S	0	0	0
			2306	1489	378	428	11			

There are 44 discrepancies between the modelled and reference sequences:

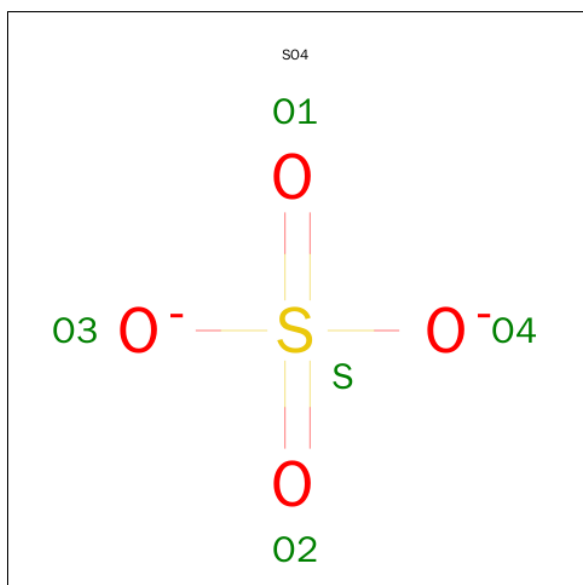
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP O25583
A	0	SER	-	expression tag	UNP O25583
A	1	LEU	-	expression tag	UNP O25583
A	302	GLU	-	expression tag	UNP O25583
A	303	GLY	-	expression tag	UNP O25583
A	304	HIS	-	expression tag	UNP O25583
A	305	HIS	-	expression tag	UNP O25583
A	306	HIS	-	expression tag	UNP O25583
A	307	HIS	-	expression tag	UNP O25583
A	308	HIS	-	expression tag	UNP O25583
A	309	HIS	-	expression tag	UNP O25583
B	-1	MET	-	expression tag	UNP O25583
B	0	SER	-	expression tag	UNP O25583
B	1	LEU	-	expression tag	UNP O25583
B	302	GLU	-	expression tag	UNP O25583
B	303	GLY	-	expression tag	UNP O25583
B	304	HIS	-	expression tag	UNP O25583
B	305	HIS	-	expression tag	UNP O25583
B	306	HIS	-	expression tag	UNP O25583
B	307	HIS	-	expression tag	UNP O25583
B	308	HIS	-	expression tag	UNP O25583

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Chain	Residue	Modelled	Actual	Comment	Reference
B	309	HIS	-	expression tag	UNP O25583
C	-1	MET	-	expression tag	UNP O25583
C	0	SER	-	expression tag	UNP O25583
C	1	LEU	-	expression tag	UNP O25583
C	302	GLU	-	expression tag	UNP O25583
C	303	GLY	-	expression tag	UNP O25583
C	304	HIS	-	expression tag	UNP O25583
C	305	HIS	-	expression tag	UNP O25583
C	306	HIS	-	expression tag	UNP O25583
C	307	HIS	-	expression tag	UNP O25583
C	308	HIS	-	expression tag	UNP O25583
C	309	HIS	-	expression tag	UNP O25583
D	-1	MET	-	expression tag	UNP O25583
D	0	SER	-	expression tag	UNP O25583
D	1	LEU	-	expression tag	UNP O25583
D	302	GLU	-	expression tag	UNP O25583
D	303	GLY	-	expression tag	UNP O25583
D	304	HIS	-	expression tag	UNP O25583
D	305	HIS	-	expression tag	UNP O25583
D	306	HIS	-	expression tag	UNP O25583
D	307	HIS	-	expression tag	UNP O25583
D	308	HIS	-	expression tag	UNP O25583
D	309	HIS	-	expression tag	UNP O25583

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

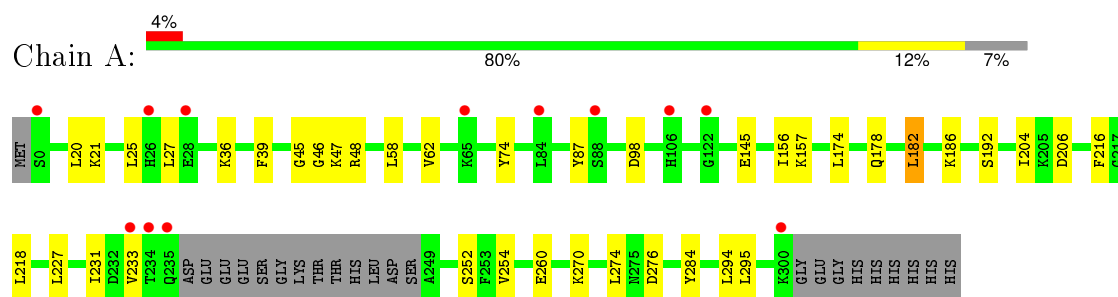
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total	O	0	0
			52	52		
3	B	50	Total	O	0	0
			50	50		
3	C	29	Total	O	0	0
			29	29		
3	D	38	Total	O	0	0
			38	38		

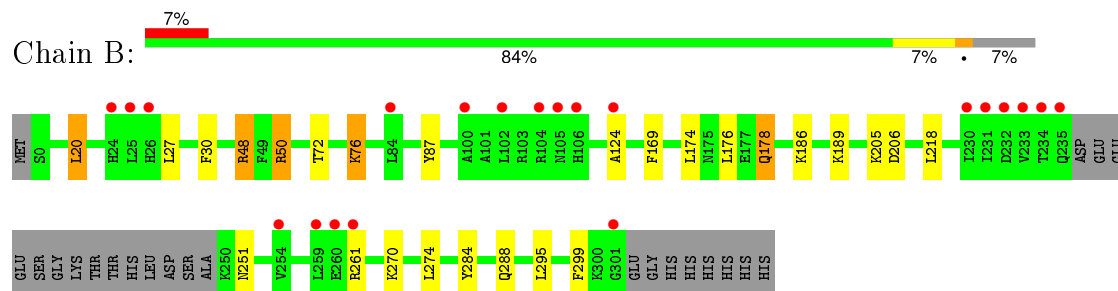
3 Residue-property plots [i](#)

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

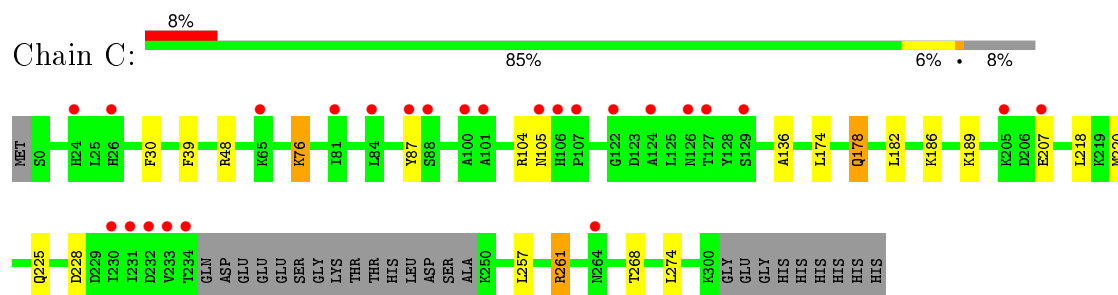
• Molecule 1: Geranyltranstransferase (IspA)



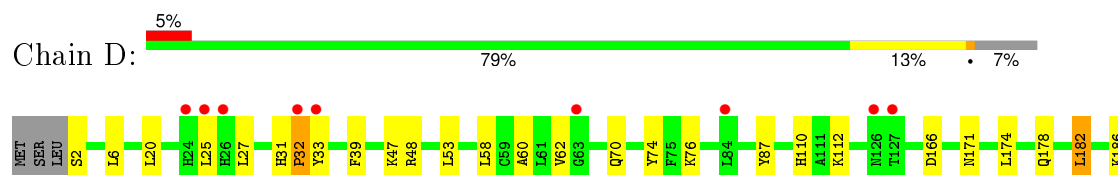
• Molecule 1: Geranyltranstransferase (IspA)

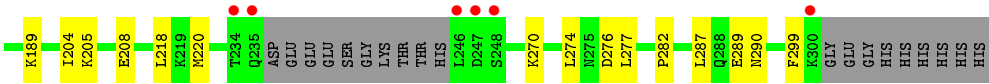


• Molecule 1: Geranyltranstransferase (IspA)



• Molecule 1: Geranyltranstransferase (IspA)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.04Å 123.84Å 111.62Å 90.00° 92.67° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 33.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.30) 98.5 (33.82-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.196 , 0.252 0.195 , 0.248	Depositor DCC
R_{free} test set	2111 reflections (3.11%)	DCC
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.8	EDS
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 70167 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9399	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.50	0/2345	0.65	2/3173 (0.1%)
1	B	0.50	0/2344	0.63	0/3171
1	C	0.47	0/2331	0.60	0/3154
1	D	0.48	0/2353	0.62	0/3184
All	All	0.49	0/9373	0.62	2/12682 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	46	GLY	N-CA-C	5.87	127.77	113.10
1	A	182	LEU	CA-CB-CG	5.77	128.58	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	GLY	Peptide
1	D	32	PRO	Peptide

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	2298	0	2307	11	0
1	B	2297	0	2305	16	0
1	C	2284	0	2294	8	0
1	D	2306	0	2308	16	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	52	0	0	0	0
3	B	50	0	0	1	0
3	C	29	0	0	0	0
3	D	38	0	0	1	0
All	All	9399	0	9214	47	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 3.

All (47) 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:20:LEU:HD12	1:B:20:LEU:C	1.82	1.01
1:B:20:LEU:HD12	1:B:20:LEU:O	1.65	0.96
1:D:31:HIS:ND1	1:D:32:PRO:HD2	1.94	0.82
1:D:31:HIS:CG	1:D:32:PRO:HD2	2.15	0.82
1:D:47:LYS:O	1:D:48:ARG:HB2	1.81	0.79
1:D:31:HIS:HE1	1:D:33:TYR:CE1	2.04	0.76
1:C:174:LEU:HB3	1:C:178:GLN:HG3	1.75	0.69
1:B:20:LEU:CD1	1:B:20:LEU:C	2.57	0.68
1:D:20:LEU:HD23	1:D:20:LEU:C	2.19	0.62
1:C:104:ARG:O	1:C:105:ASN:HB2	2.02	0.59
1:B:174:LEU:HB3	1:B:178:GLN:HG3	1.88	0.56
1:B:20:LEU:HD21	1:B:48:ARG:NH1	2.21	0.56
1:D:32:PRO:HG2	1:D:33:TYR:CD2	2.43	0.53
1:C:257:LEU:HB3	1:C:261:ARG:HB3	1.92	0.52
1:A:174:LEU:HB3	1:A:178:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:O	1:A:231:ILE:HG12	2.10	0.51
1:B:50:ARG:NH2	3:B:322:HOH:O	2.43	0.50
1:A:233:VAL:HG21	1:A:254:VAL:HG11	1.95	0.49
1:D:31:HIS:ND1	1:D:32:PRO:CD	2.74	0.48
1:A:178:GLN:HB2	1:B:30:PHE:CZ	2.49	0.47
1:B:48:ARG:N	1:B:48:ARG:HD3	2.30	0.47
1:A:206:ASP:OD2	1:A:284:TYR:OH	2.27	0.47
1:A:20:LEU:C	1:A:20:LEU:HD23	2.34	0.47
1:A:58:LEU:O	1:A:62:VAL:HG12	2.16	0.46
1:A:156:ILE:HB	1:B:124:ALA:HB1	1.96	0.46
1:C:178:GLN:HB3	1:C:178:GLN:HE21	1.61	0.46
1:A:178:GLN:HB2	1:B:30:PHE:CE2	2.51	0.46
1:D:174:LEU:HB3	1:D:178:GLN:HG3	1.98	0.45
1:A:216:PHE:HZ	1:A:295:LEU:HD11	1.82	0.45
1:B:169:PHE:O	1:B:251:ASN:ND2	2.50	0.44
1:D:58:LEU:HD21	1:D:74:TYR:CG	2.53	0.44
1:C:76:LYS:HE2	1:C:136:ALA:HA	2.00	0.44
1:D:32:PRO:CG	1:D:33:TYR:CD2	3.00	0.44
1:D:6:LEU:HD13	1:D:289:GLU:HG2	1.99	0.44
1:D:166:ASP:HB2	1:D:182:LEU:HD11	2.01	0.43
1:C:104:ARG:O	1:C:105:ASN:CB	2.66	0.43
1:C:30:PHE:CZ	1:D:178:GLN:HB2	2.54	0.43
1:D:110:HIS:HD2	3:D:314:HOH:O	2.01	0.42
1:B:206:ASP:OD2	1:B:284:TYR:OH	2.31	0.42
1:B:295:LEU:HA	1:B:295:LEU:HD23	1.90	0.42
1:C:182:LEU:HD23	1:C:182:LEU:C	2.41	0.42
1:B:270:LYS:HE3	1:B:299:PHE:HB3	2.03	0.41
1:D:60:ALA:HB2	1:D:290:ASN:ND2	2.36	0.41
1:B:72:THR:O	1:B:76:LYS:HG2	2.21	0.41
1:B:178:GLN:HE21	1:B:178:GLN:HB3	1.62	0.40
1:A:58:LEU:HD21	1:A:74:TYR:CG	2.57	0.40
1:D:270:LYS:HE3	1:D:299:PHE:HB3	2.02	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	284/311 (91%)	279 (98%)	5 (2%)	0	100	100
1	B	284/311 (91%)	274 (96%)	10 (4%)	0	100	100
1	C	282/311 (91%)	276 (98%)	6 (2%)	0	100	100
1	D	285/311 (92%)	279 (98%)	5 (2%)	1 (0%)	39	48
All	All	1135/1244 (91%)	1108 (98%)	26 (2%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	282	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/273 (93%)	231 (91%)	22 (9%)	13	15
1	B	253/273 (93%)	238 (94%)	15 (6%)	24	32
1	C	252/273 (92%)	237 (94%)	15 (6%)	24	31
1	D	254/273 (93%)	231 (91%)	23 (9%)	12	13
All	All	1012/1092 (93%)	937 (93%)	75 (7%)	17	21

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	25	LEU
1	A	27	LEU
1	A	36	LYS
1	A	39	PHE

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Mol	Chain	Res	Type
1	A	47	LYS
1	A	48	ARG
1	A	87	TYR
1	A	98	ASP
1	A	145	GLU
1	A	157	LYS
1	A	182	LEU
1	A	186	LYS
1	A	192	SER
1	A	204	ILE
1	A	218	LEU
1	A	252	SER
1	A	260	GLU
1	A	270	LYS
1	A	274	LEU
1	A	276	ASP
1	A	294	LEU
1	B	20	LEU
1	B	27	LEU
1	B	48	ARG
1	B	50	ARG
1	B	76	LYS
1	B	87	TYR
1	B	176	LEU
1	B	178	GLN
1	B	186	LYS
1	B	189	LYS
1	B	205	LYS
1	B	218	LEU
1	B	261	ARG
1	B	274	LEU
1	B	288	GLN
1	C	39	PHE
1	C	48	ARG
1	C	76	LYS
1	C	87	TYR
1	C	178	GLN
1	C	186	LYS
1	C	189	LYS
1	C	207	GLU
1	C	218	LEU
1	C	220	MET

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Mol	Chain	Res	Type
1	C	225	GLN
1	C	228	ASP
1	C	261	ARG
1	C	268	THR
1	C	274	LEU
1	D	2	SER
1	D	25	LEU
1	D	27	LEU
1	D	39	PHE
1	D	53	LEU
1	D	62	VAL
1	D	70	GLN
1	D	76	LYS
1	D	87	TYR
1	D	112	LYS
1	D	171	ASN
1	D	182	LEU
1	D	186	LYS
1	D	189	LYS
1	D	204	ILE
1	D	205	LYS
1	D	208	GLU
1	D	218	LEU
1	D	220	MET
1	D	274	LEU
1	D	276	ASP
1	D	277	LEU
1	D	287	LEU

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

Mol	Chain	Res	Type
1	A	44	ASN
1	A	235	GLN
1	B	288	GLN
1	C	178	GLN
1	C	288	GLN
1	D	31	HIS
1	D	64	GLN
1	D	99	ASN
1	D	214	GLN
1	D	264	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
2	SO4	A	310	-	4,4,4	0.11	0	6,6,6	0.10	0
2	SO4	A	311	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	B	310	-	4,4,4	0.20	0	6,6,6	0.18	0
2	SO4	B	311	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	B	312	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	C	310	-	4,4,4	0.11	0	6,6,6	0.13	0
2	SO4	C	311	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	D	310	-	4,4,4	0.30	0	6,6,6	0.20	0
2	SO4	D	311	-	4,4,4	0.20	0	6,6,6	0.19	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	SO4	A	310	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	311	-	-	0/0/0/0	0/0/0/0
2	SO4	B	310	-	-	0/0/0/0	0/0/0/0
2	SO4	B	311	-	-	0/0/0/0	0/0/0/0
2	SO4	B	312	-	-	0/0/0/0	0/0/0/0
2	SO4	C	310	-	-	0/0/0/0	0/0/0/0
2	SO4	C	311	-	-	0/0/0/0	0/0/0/0
2	SO4	D	310	-	-	0/0/0/0	0/0/0/0
2	SO4	D	311	-	-	0/0/0/0	0/0/0/0

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	288/311 (92%)	0.15	12 (4%)	40 49	34, 52, 85, 131	0
1	B	288/311 (92%)	0.29	21 (7%)	18 25	28, 52, 87, 129	0
1	C	286/311 (91%)	0.44	25 (8%)	13 18	36, 57, 96, 138	0
1	D	289/311 (92%)	0.28	15 (5%)	31 39	35, 59, 97, 135	0
All	All	1151/1244 (92%)	0.29	73 (6%)	23 31	28, 55, 93, 138	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	234	THR	9.2
1	A	234	THR	6.9
1	B	235	GLN	6.1
1	A	235	GLN	5.7
1	B	234	THR	5.1
1	D	235	GLN	5.0
1	D	234	THR	4.9
1	C	230	ILE	4.6
1	C	106	HIS	4.5
1	B	105	ASN	4.2
1	B	254	VAL	4.2
1	C	127	THR	4.0
1	D	246	LEU	4.0
1	C	231	ILE	3.8
1	B	232	ASP	3.8
1	C	26	HIS	3.7
1	B	301	GLY	3.7
1	C	233	VAL	3.6
1	D	24	HIS	3.6
1	B	26	HIS	3.5
1	A	233	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	84	LEU	3.5
1	A	26	HIS	3.5
1	A	0	SER	3.4
1	D	25	LEU	3.4
1	B	24	HIS	3.2
1	D	26	HIS	3.2
1	B	25	LEU	3.1
1	D	84	LEU	3.0
1	C	105	ASN	3.0
1	B	260	GLU	3.0
1	A	65	LYS	2.9
1	C	205	LYS	2.9
1	C	124	ALA	2.9
1	A	84	LEU	2.9
1	B	84	LEU	2.9
1	B	100	ALA	2.8
1	C	88	SER	2.8
1	C	87	TYR	2.7
1	B	259	LEU	2.7
1	A	300	LYS	2.7
1	C	101	ALA	2.7
1	A	122	GLY	2.7
1	A	106	HIS	2.6
1	C	24	HIS	2.6
1	C	232	ASP	2.6
1	C	122	GLY	2.6
1	C	81	ILE	2.6
1	B	106	HIS	2.5
1	B	233	VAL	2.5
1	D	33	TYR	2.5
1	C	107	PRO	2.5
1	D	127	THR	2.5
1	B	104	ARG	2.5
1	C	207	GLU	2.4
1	B	230	ILE	2.4
1	C	65	LYS	2.4
1	B	261	ARG	2.4
1	D	300	LYS	2.4
1	D	248	SER	2.3
1	C	129	SER	2.3
1	A	28	GLU	2.3
1	A	88	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	126	ASN	2.3
1	C	100	ALA	2.2
1	C	264	ASN	2.2
1	D	32	PRO	2.1
1	D	126	ASN	2.1
1	D	247	ASP	2.1
1	B	231	ILE	2.1
1	B	124	ALA	2.1
1	D	63	GLY	2.0
1	B	102	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	311	5/5	0.72	0.21	1.47	79,96,105,106	0
2	SO4	C	311	5/5	0.97	0.14	0.62	81,83,88,90	0
2	SO4	D	311	5/5	0.92	0.10	-0.83	103,105,108,109	0
2	SO4	A	310	5/5	0.97	0.09	-1.21	67,70,72,75	0
2	SO4	D	310	5/5	0.92	0.13	-1.49	95,98,100,100	0
2	SO4	B	311	5/5	0.94	0.08	-1.89	55,57,78,79	0
2	SO4	B	310	5/5	0.98	0.08	-2.13	60,62,65,66	0
2	SO4	C	310	5/5	0.94	0.10	-2.17	79,80,87,89	0
2	SO4	B	312	5/5	0.90	0.12	-	122,124,125,127	0

6.5 Other polymers

There are no such residues in this entry.