



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:15 AM GMT

PDB ID : 3DWK
Title : Identification of Dynamic Structural Motifs Involved in Peptidoglycan Glycosyltransfer
Authors : Lovering, A.L.; De Castro, L.; Strynadka, N.C.J.
Deposited on : 2008-07-22
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

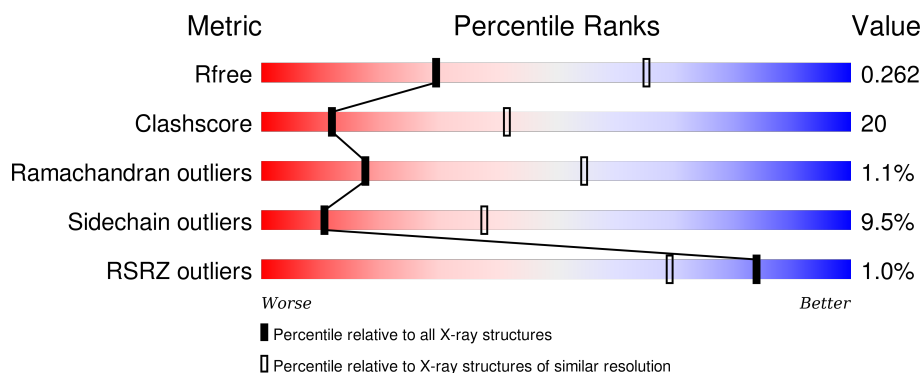
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	625	<div> <div>2%</div> <div>57% 34% . .</div> </div>
1	B	625	<div> <div>%</div> <div>62% 32% . .</div> </div>
1	C	625	<div> <div>61% 34% 5%</div> </div>
1	D	625	<div> <div>60% 32% . .</div> </div>

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	SO4	A	11	-	-	X	-
2	SO4	A	15	-	-	X	-
2	SO4	A	17	-	-	X	-
2	SO4	A	27	-	-	-	X
2	SO4	A	41	-	-	X	-
2	SO4	B	38	-	-	X	-
2	SO4	C	31	-	-	X	-
2	SO4	D	39	-	-	X	-
3	LDA	D	1	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19474 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.

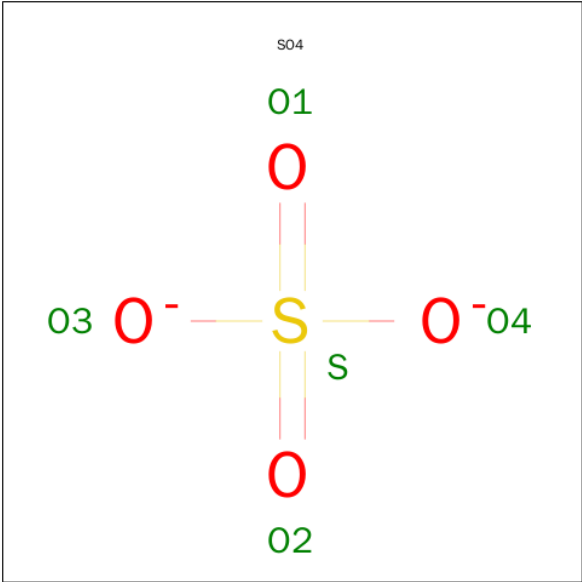
- Molecule 1 is a protein called Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4712	2953	809	938	12			
1	B	621	Total	C	N	O	S	0	0	0
			4874	3051	839	972	12			
1	C	623	Total	C	N	O	S	0	0	0
			4891	3060	843	976	12			
1	D	602	Total	C	N	O	S	0	0	0
			4751	2977	817	945	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	MET	LYS	ENGINEERED	UNP Q5HFX3
B	68	MET	LYS	ENGINEERED	UNP Q5HFX3
C	68	MET	LYS	ENGINEERED	UNP Q5HFX3
D	68	MET	LYS	ENGINEERED	UNP Q5HFX3

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



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

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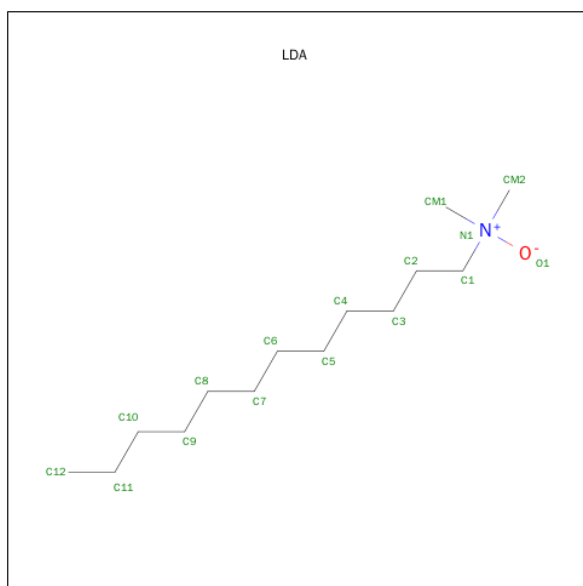
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

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

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

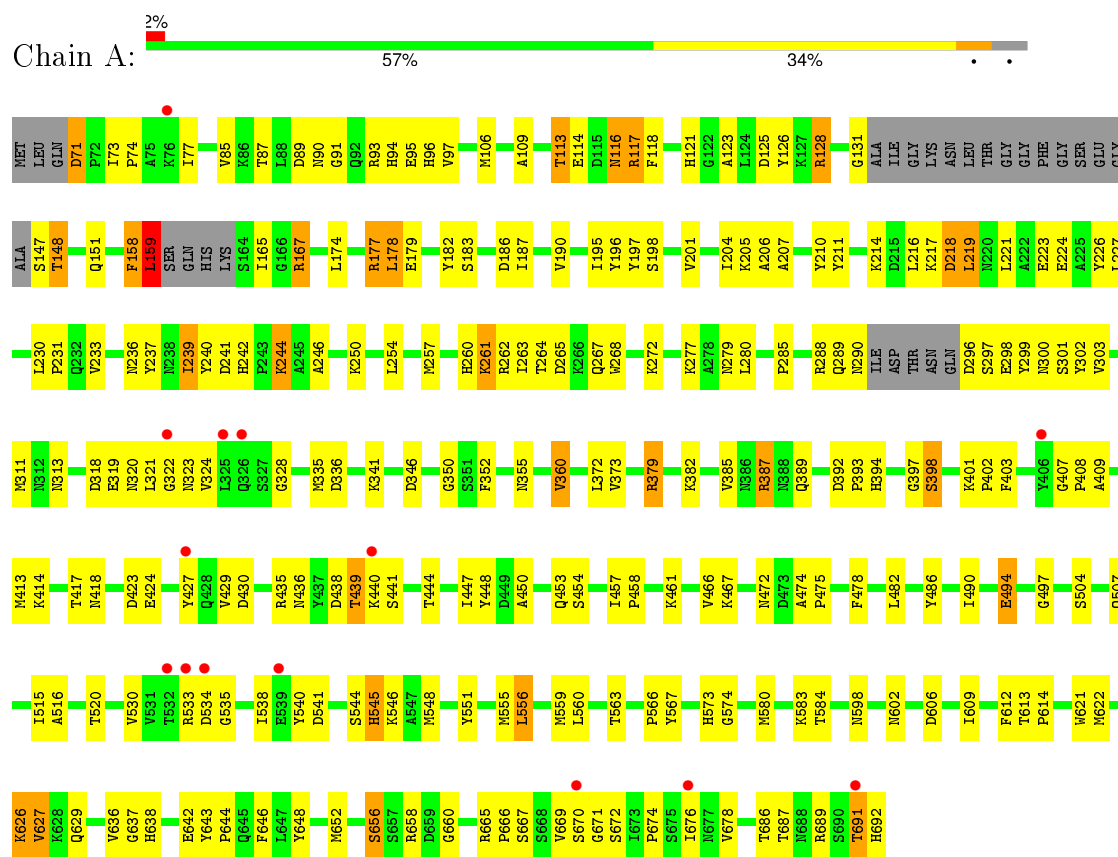


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			16	14	1	1		

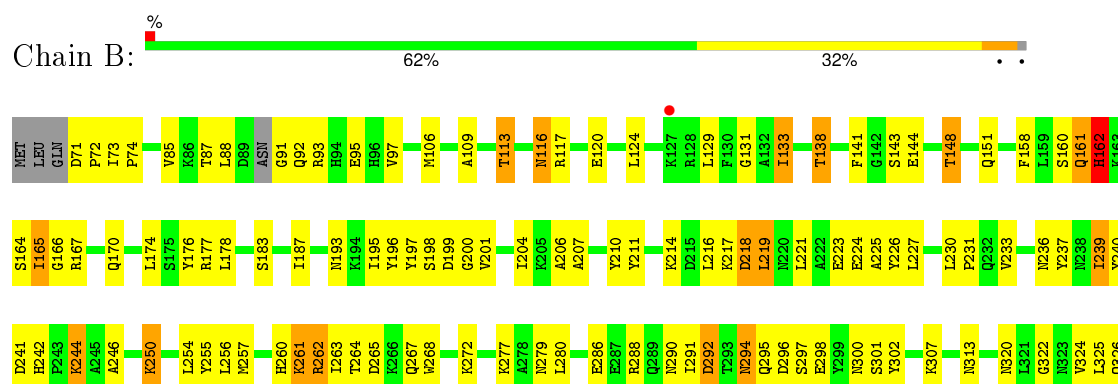
3 Residue-property plots [i](#)

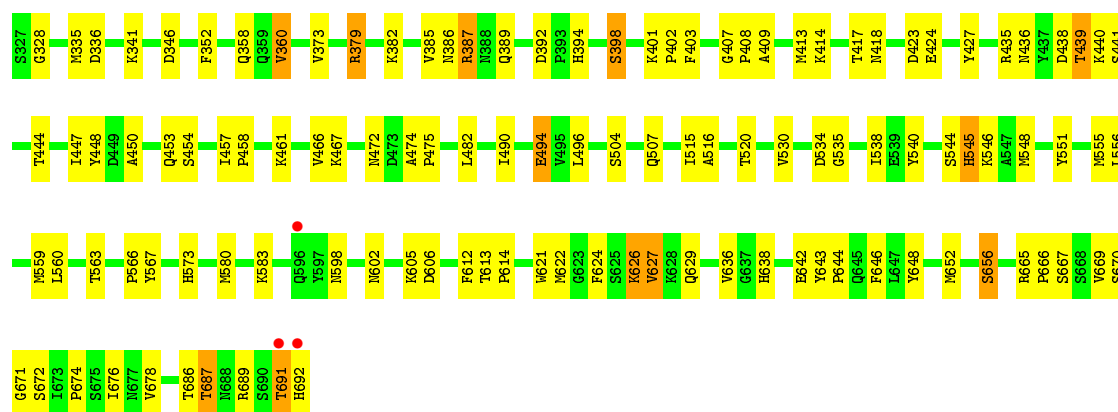
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Penicillin-binding protein 2



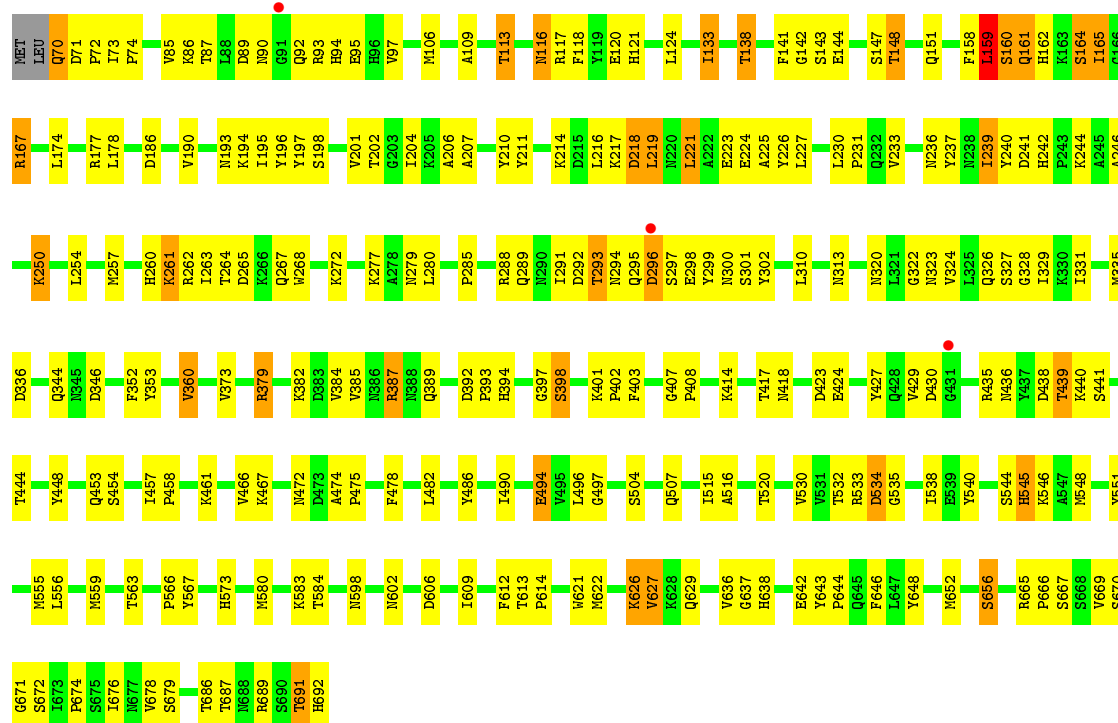
- Molecule 1: Penicillin-binding protein 2





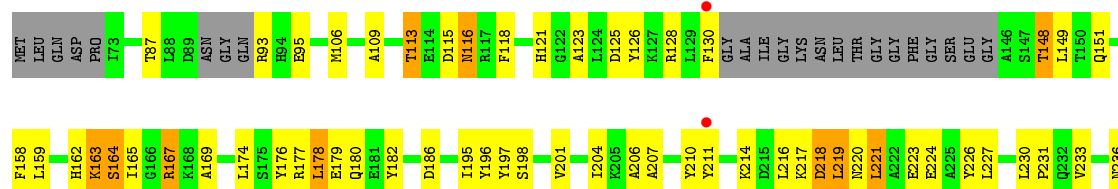
• Molecule 1: Penicillin-binding protein 2

Chain C: 61% 34% 5%



• Molecule 1: Penicillin-binding protein 2

Chain D: 60% 32%



P644	Q645	R646	L647	Y648	M652	S656	R665	P666	S667	S668	V669	S670	G671	S672	I673	P674	S675	I676	N677	V678	S679	T686	T687	N688	R689	S690	T691	H692																				
I538	E539	Y540	S544	H545	K546	A547	M548	Y551	M555	L556	M559	L560	T563	P566	Y567	A570	H573	G574	M580	K583	N598	M602	K605	D606	V607	M610	G611	F612	T613	P614	W621	M622	K626	V627	R628	Q629	V636	G637	H638	E642	Y643							
M436	T437	D438	T439	K440	S441	T444	I447	Y448	D449	A450	Q453	S454	T457	P458	K461	Y466	K467	M472	D473	A474	P475	F478	L482	Y486	I490	E494	S504	Q507	T515	A516	T520	M523	A524	H525	V530	V531	T532	R533	D534	G535								
Y237	H238	I239	Y240	D241	H242	P243	K244	A245	A246	K250	L254	M257	H260	K261	I262	I263	T264	D265	K266	Q267	N268	K272	K277	A278	I279	L280	R288	Q289	M290	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323
V324	I331	M335	D336	K341	Q344	D346	G350	S351	F352	V360	V373	R379	K382	D383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	K401	P402	F403	P408	A409	M413	K414	T417	M418	D423	E424	Y427	Q428	V429	D430	R435								

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.35Å 217.47Å 95.73Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	41.88 – 3.10 41.88 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (41.88-3.10) 94.4 (41.88-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.12Å)	Xtriage
Refinement program	REFMAC5	Depositor
R, R_{free}	0.218 , 0.264 0.217 , 0.262	Depositor DCC
R_{free} test set	3052 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.125 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 60418 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19474	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: LDA, 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	0.36	0/4813	0.53	2/6504 (0.0%)
1	B	0.35	0/4979	0.51	0/6729
1	C	0.38	0/4997	0.54	1/6755 (0.0%)
1	D	0.37	0/4853	0.53	0/6559
All	All	0.37	0/19642	0.53	3/26547 (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	C	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	LEU	CA-CB-CG	-7.58	97.86	115.30
1	A	131	GLY	N-CA-C	-6.72	96.29	113.10
1	A	159	LEU	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	C	159	LEU	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	4712	0	4518	190	0
1	B	4874	0	4676	191	0
1	C	4891	0	4691	208	0
1	D	4751	0	4562	185	0
2	A	75	0	0	14	0
2	B	65	0	0	8	0
2	C	45	0	0	6	0
2	D	45	0	0	5	0
3	D	16	0	31	7	0
All	All	19474	0	18478	759	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 20.

The worst 5 of 759 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:162:HIS:CE1	1:B:164:SER:HB2	1.78	1.18
1:C:160:SER:HB2	1:C:167:ARG:NH1	1.61	1.15
1:C:160:SER:CB	1:C:167:ARG:HH11	1.59	1.14
1:C:159:LEU:HD22	1:C:532:THR:HB	1.23	1.11
1:D:118:PHE:HA	1:D:121:HIS:CE1	1.95	1.01

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	590/625 (94%)	534 (90%)	50 (8%)	6 (1%)	19	58
1	B	617/625 (99%)	565 (92%)	46 (8%)	6 (1%)	19	58
1	C	621/625 (99%)	563 (91%)	50 (8%)	8 (1%)	15	50
1	D	596/625 (95%)	545 (91%)	45 (8%)	6 (1%)	19	58
All	All	2424/2500 (97%)	2207 (91%)	191 (8%)	26 (1%)	17	55

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	SER
1	B	162	HIS
1	B	292	ASP
1	C	143	SER
1	C	160	SER

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	506/526 (96%)	457 (90%)	49 (10%)	10	36
1	B	522/526 (99%)	472 (90%)	50 (10%)	10	37
1	C	524/526 (100%)	474 (90%)	50 (10%)	11	38
1	D	511/526 (97%)	464 (91%)	47 (9%)	11	40
All	All	2063/2104 (98%)	1867 (90%)	196 (10%)	11	38

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	563	THR
1	C	164	SER
1	D	494	GLU
1	B	627	VAL
1	C	70	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	92	GLN
1	C	279	ASN
1	D	472	ASN
1	C	94	HIS
1	C	121	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

47 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	11	-	4,4,4	0.14	0	6,6,6	0.37	0
2	SO4	A	12	-	4,4,4	0.17	0	6,6,6	0.20	0
2	SO4	A	15	-	4,4,4	0.24	0	6,6,6	0.29	0
2	SO4	A	16	-	4,4,4	0.16	0	6,6,6	0.17	0
2	SO4	A	17	-	4,4,4	0.24	0	6,6,6	0.25	0
2	SO4	A	22	-	4,4,4	0.20	0	6,6,6	0.16	0
2	SO4	A	24	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	A	26	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	A	27	-	4,4,4	0.18	0	6,6,6	0.17	0
2	SO4	A	29	-	4,4,4	0.18	0	6,6,6	0.12	0
2	SO4	A	3	-	4,4,4	0.23	0	6,6,6	0.30	0
2	SO4	A	41	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	A	43	-	4,4,4	0.17	0	6,6,6	0.23	0
2	SO4	A	45	-	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	A	46	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	B	20	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	B	21	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	B	23	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	B	25	-	4,4,4	0.15	0	6,6,6	0.23	0
2	SO4	B	32	-	4,4,4	0.18	0	6,6,6	0.19	0
2	SO4	B	34	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	B	35	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	B	36	-	4,4,4	0.24	0	6,6,6	0.31	0
2	SO4	B	37	-	4,4,4	0.18	0	6,6,6	0.11	0
2	SO4	B	38	-	4,4,4	0.21	0	6,6,6	0.38	0
2	SO4	B	42	-	4,4,4	0.17	0	6,6,6	0.17	0
2	SO4	B	44	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	B	8	-	4,4,4	0.17	0	6,6,6	0.24	0
2	SO4	C	1	-	4,4,4	0.22	0	6,6,6	0.28	0
2	SO4	C	18	-	4,4,4	0.18	0	6,6,6	0.22	0
2	SO4	C	19	-	4,4,4	0.12	0	6,6,6	0.52	0
2	SO4	C	2	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	C	28	-	4,4,4	0.20	0	6,6,6	0.27	0
2	SO4	C	31	-	4,4,4	0.19	0	6,6,6	0.35	0
2	SO4	C	33	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	C	4	-	4,4,4	0.17	0	6,6,6	0.36	0
2	SO4	C	6	-	4,4,4	0.12	0	6,6,6	0.18	0
3	LDA	D	1	-	15,15,15	3.92	2 (13%)	16,17,17	0.77	0
2	SO4	D	10	-	4,4,4	0.23	0	6,6,6	0.18	0
2	SO4	D	13	-	4,4,4	0.13	0	6,6,6	0.30	0
2	SO4	D	14	-	4,4,4	0.21	0	6,6,6	0.25	0
2	SO4	D	30	-	4,4,4	0.17	0	6,6,6	0.06	0
2	SO4	D	39	-	4,4,4	0.17	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	40	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SO4	D	5	-	4,4,4	0.22	0	6,6,6	0.32	0
2	SO4	D	7	-	4,4,4	0.19	0	6,6,6	0.20	0
2	SO4	D	9	-	4,4,4	0.15	0	6,6,6	0.23	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	11	-	-	0/0/0/0	0/0/0/0
2	SO4	A	12	-	-	0/0/0/0	0/0/0/0
2	SO4	A	15	-	-	0/0/0/0	0/0/0/0
2	SO4	A	16	-	-	0/0/0/0	0/0/0/0
2	SO4	A	17	-	-	0/0/0/0	0/0/0/0
2	SO4	A	22	-	-	0/0/0/0	0/0/0/0
2	SO4	A	24	-	-	0/0/0/0	0/0/0/0
2	SO4	A	26	-	-	0/0/0/0	0/0/0/0
2	SO4	A	27	-	-	0/0/0/0	0/0/0/0
2	SO4	A	29	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	A	41	-	-	0/0/0/0	0/0/0/0
2	SO4	A	43	-	-	0/0/0/0	0/0/0/0
2	SO4	A	45	-	-	0/0/0/0	0/0/0/0
2	SO4	A	46	-	-	0/0/0/0	0/0/0/0
2	SO4	B	20	-	-	0/0/0/0	0/0/0/0
2	SO4	B	21	-	-	0/0/0/0	0/0/0/0
2	SO4	B	23	-	-	0/0/0/0	0/0/0/0
2	SO4	B	25	-	-	0/0/0/0	0/0/0/0
2	SO4	B	32	-	-	0/0/0/0	0/0/0/0
2	SO4	B	34	-	-	0/0/0/0	0/0/0/0
2	SO4	B	35	-	-	0/0/0/0	0/0/0/0
2	SO4	B	36	-	-	0/0/0/0	0/0/0/0
2	SO4	B	37	-	-	0/0/0/0	0/0/0/0
2	SO4	B	38	-	-	0/0/0/0	0/0/0/0
2	SO4	B	42	-	-	0/0/0/0	0/0/0/0
2	SO4	B	44	-	-	0/0/0/0	0/0/0/0
2	SO4	B	8	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1	-	-	0/0/0/0	0/0/0/0
2	SO4	C	18	-	-	0/0/0/0	0/0/0/0
2	SO4	C	19	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	28	-	-	0/0/0/0	0/0/0/0
2	SO4	C	31	-	-	0/0/0/0	0/0/0/0
2	SO4	C	33	-	-	0/0/0/0	0/0/0/0
2	SO4	C	4	-	-	0/0/0/0	0/0/0/0
2	SO4	C	6	-	-	0/0/0/0	0/0/0/0
3	LDA	D	1	-	-	0/13/13/13	0/0/0/0
2	SO4	D	10	-	-	0/0/0/0	0/0/0/0
2	SO4	D	13	-	-	0/0/0/0	0/0/0/0
2	SO4	D	14	-	-	0/0/0/0	0/0/0/0
2	SO4	D	30	-	-	0/0/0/0	0/0/0/0
2	SO4	D	39	-	-	0/0/0/0	0/0/0/0
2	SO4	D	40	-	-	0/0/0/0	0/0/0/0
2	SO4	D	5	-	-	0/0/0/0	0/0/0/0
2	SO4	D	7	-	-	0/0/0/0	0/0/0/0
2	SO4	D	9	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	LDA	O1-N1	-14.72	1.25	1.39
3	D	1	LDA	C1-N1	-3.32	1.45	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	11	SO4	2	0
2	A	15	SO4	2	0
2	A	17	SO4	4	0
2	A	3	SO4	1	0
2	A	41	SO4	5	0
2	B	23	SO4	1	0
2	B	25	SO4	1	0
2	B	35	SO4	1	0
2	B	38	SO4	5	0
2	C	18	SO4	1	0
2	C	19	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	31	SO4	3	0
2	C	4	SO4	1	0
3	D	1	LDA	7	0
2	D	39	SO4	2	0
2	D	5	SO4	1	0
2	D	7	SO4	1	0
2	D	9	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 [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	598/625 (95%)	0.22	14 (2%) 64 40	30, 74, 136, 217	0
1	B	621/625 (99%)	0.11	4 (0%) 90 80	24, 68, 118, 219	0
1	C	623/625 (99%)	0.06	3 (0%) 91 83	14, 60, 112, 317	0
1	D	602/625 (96%)	0.09	3 (0%) 91 83	24, 64, 129, 183	0
All	All	2444/2500 (97%)	0.12	24 (0%) 84 69	14, 66, 125, 317	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	GLY	4.3
1	B	691	THR	3.4
1	B	692	HIS	3.3
1	D	130	PHE	3.1
1	A	326	GLN	3.0

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
3	LDA	D	1	16/16	0.97	0.42	3.73	49,49,49,49	0
2	SO4	A	27	5/5	0.88	0.30	2.37	101,101,101,101	0
2	SO4	D	14	5/5	0.93	0.22	0.51	105,105,105,105	0
2	SO4	A	15	5/5	0.98	0.21	-0.34	50,50,50,50	0
2	SO4	C	4	5/5	0.93	0.20	-0.43	79,79,79,79	0
2	SO4	D	9	5/5	0.94	0.18	-0.55	75,75,75,75	0
2	SO4	A	46	5/5	0.90	0.21	-0.65	151,151,151,151	0
2	SO4	C	1	5/5	0.97	0.18	-0.70	82,82,82,82	0
2	SO4	A	26	5/5	0.97	0.17	-0.80	101,101,101,101	0
2	SO4	A	3	5/5	0.97	0.17	-0.94	79,79,79,79	0
2	SO4	A	41	5/5	0.93	0.19	-0.97	91,91,91,91	0
2	SO4	A	45	5/5	0.96	0.15	-1.13	115,115,115,115	0
2	SO4	C	19	5/5	0.97	0.16	-1.13	58,58,58,58	0
2	SO4	D	30	5/5	0.96	0.16	-1.21	112,112,112,112	0
2	SO4	B	8	5/5	0.98	0.16	-1.54	70,70,70,70	0
2	SO4	D	10	5/5	0.98	0.18	-1.68	53,53,53,53	0
2	SO4	B	34	5/5	0.97	0.19	-1.90	69,69,69,69	0
2	SO4	A	24	5/5	0.94	0.18	-1.96	79,79,79,79	0
2	SO4	D	5	5/5	0.96	0.15	-2.14	85,85,85,85	0
2	SO4	B	42	5/5	0.95	0.15	-2.20	94,94,94,94	0
2	SO4	B	32	5/5	0.92	0.17	-2.25	104,104,104,104	0
2	SO4	B	44	5/5	0.95	0.12	-2.40	118,118,118,118	0
2	SO4	C	33	5/5	0.93	0.16	-2.48	101,101,101,101	0
2	SO4	A	16	5/5	0.90	0.14	-2.62	108,108,108,108	0
2	SO4	A	11	5/5	0.94	0.12	-2.70	90,90,90,90	0
2	SO4	A	43	5/5	0.83	0.18	-2.85	129,129,129,129	0
2	SO4	B	23	5/5	0.97	0.11	-3.22	95,95,95,95	0
2	SO4	C	6	5/5	0.98	0.14	-3.28	77,77,77,77	0
2	SO4	B	35	5/5	0.97	0.12	-3.95	102,102,102,102	0
2	SO4	B	21	5/5	0.96	0.12	-	87,87,87,87	0
2	SO4	B	20	5/5	0.93	0.12	-	119,119,119,119	0
2	SO4	D	13	5/5	0.93	0.16	-	102,102,102,102	0
2	SO4	A	29	5/5	0.97	0.08	-	112,112,112,112	0
2	SO4	A	17	5/5	0.97	0.15	-	88,88,88,88	0
2	SO4	A	12	5/5	0.92	0.20	-	108,108,108,108	0
2	SO4	B	38	5/5	0.96	0.12	-	91,91,91,91	0
2	SO4	C	18	5/5	0.98	0.12	-	75,75,75,75	0
2	SO4	C	2	5/5	0.88	0.18	-	106,106,106,106	0
2	SO4	D	7	5/5	0.99	0.14	-	81,81,81,81	0
2	SO4	B	25	5/5	0.95	0.12	-	100,100,100,100	0
2	SO4	C	28	5/5	0.89	0.17	-	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	36	5/5	0.93	0.18	-	94,94,94,94	0
2	SO4	D	39	5/5	0.88	0.12	-	123,123,123,123	0
2	SO4	B	37	5/5	0.86	0.17	-	123,123,123,123	0
2	SO4	C	31	5/5	0.93	0.16	-	81,81,81,81	0
2	SO4	D	40	5/5	0.91	0.16	-	104,104,104,104	0
2	SO4	A	22	5/5	0.94	0.14	-	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.