



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:21 PM UTC

PDB ID : 2Q4O / pdb_00002q4o
Title : Ensemble refinement of the crystal structure of a lysine decarboxylase-like protein from Arabidopsis thaliana gene At2g37210
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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:

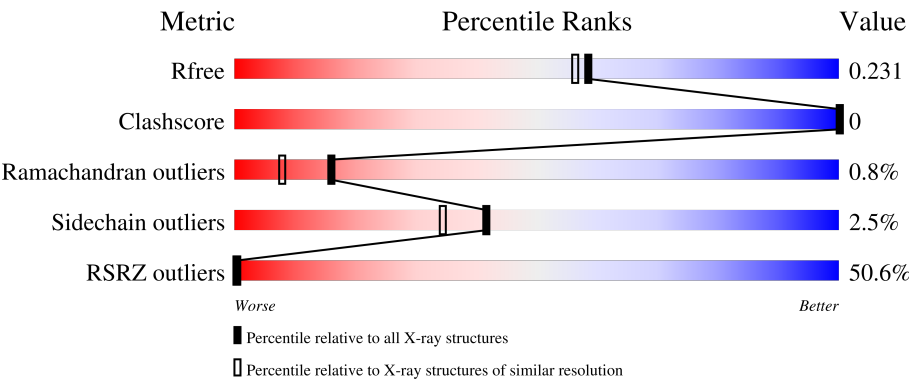
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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.



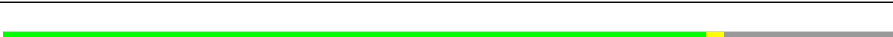
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	1-A	215	43% 80% 19%
1	1-B	215	37% 78% 20%
1	2-A	215	80% 19%
1	2-B	215	77% 20%
1	3-A	215	80% 19%

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Mol	Chain	Length	Quality of chain
1	3-B	215	 78% 20%
1	4-A	215	 80% 19%
1	4-B	215	 79% 20%
1	5-A	215	 80% 19%
1	5-B	215	 78% 20%
1	6-A	215	 80% 19%
1	6-B	215	 78% 20%
1	7-A	215	 78% 19%
1	7-B	215	 78% 20%
1	8-A	215	 78% 19%
1	8-B	215	 79% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22875 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.

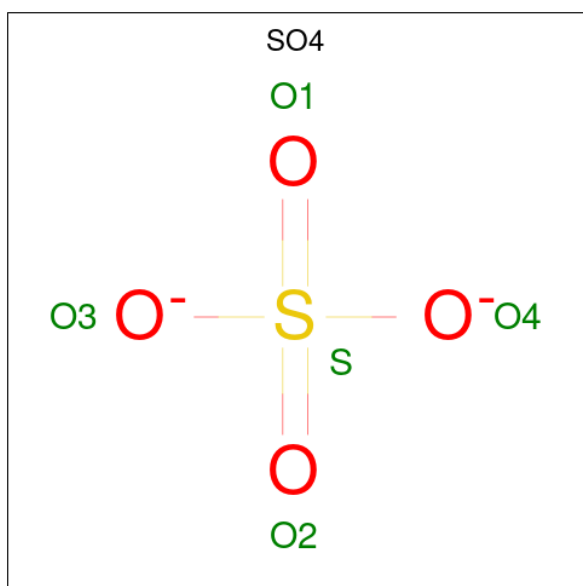
- Molecule 1 is a protein called Uncharacterized protein At2g37210/T2N18.3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	175	Total	C	N	O	S	Se	0	0	0
			1328	842	229	250	2	5			
1	2-A	175	Total	C	N	O	S	Se	0	0	0
			1328	842	229	250	2	5			
1	3-A	175	Total	C	N	O	S	Se	0	0	0
			1328	842	229	250	2	5			
1	4-A	175	Total	C	N	O	S	Se	0	0	0
			1328	842	229	250	2	5			
1	5-A	175	Total	C	N	O	S	Se	0	0	0
			1328	842	229	250	2	5			
1	6-A	175	Total	C	N	O	S	Se	0	0	0
			1328	842	229	250	2	5			
1	7-A	175	Total	C	N	O	S	Se	0	0	0
			1328	842	229	250	2	5			
1	8-A	175	Total	C	N	O	S	Se	0	0	0
			1328	842	229	250	2	5			
1	1-B	173	Total	C	N	O	S	Se	0	0	0
			1308	828	226	249	2	3			
1	2-B	173	Total	C	N	O	S	Se	0	0	0
			1308	828	226	249	2	3			
1	3-B	173	Total	C	N	O	S	Se	0	0	0
			1308	828	226	249	2	3			
1	4-B	173	Total	C	N	O	S	Se	0	0	0
			1308	828	226	249	2	3			
1	5-B	173	Total	C	N	O	S	Se	0	0	0
			1308	828	226	249	2	3			
1	6-B	173	Total	C	N	O	S	Se	0	0	0
			1308	828	226	249	2	3			
1	7-B	173	Total	C	N	O	S	Se	0	0	0
			1308	828	226	249	2	3			
1	8-B	173	Total	C	N	O	S	Se	0	0	0
			1308	828	226	249	2	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8L8B8
A	8	MSE	MET	modified residue	UNP Q8L8B8
A	58	MSE	MET	modified residue	UNP Q8L8B8
A	81	MSE	MET	modified residue	UNP Q8L8B8
A	99	MSE	MET	modified residue	UNP Q8L8B8
A	106	MSE	MET	modified residue	UNP Q8L8B8
A	206	MSE	MET	modified residue	UNP Q8L8B8
B	1	MSE	MET	modified residue	UNP Q8L8B8
B	8	MSE	MET	modified residue	UNP Q8L8B8
B	58	MSE	MET	modified residue	UNP Q8L8B8
B	81	MSE	MET	modified residue	UNP Q8L8B8
B	99	MSE	MET	modified residue	UNP Q8L8B8
B	106	MSE	MET	modified residue	UNP Q8L8B8
B	206	MSE	MET	modified residue	UNP Q8L8B8

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-B	1	Total 1	Mg 1	0	0

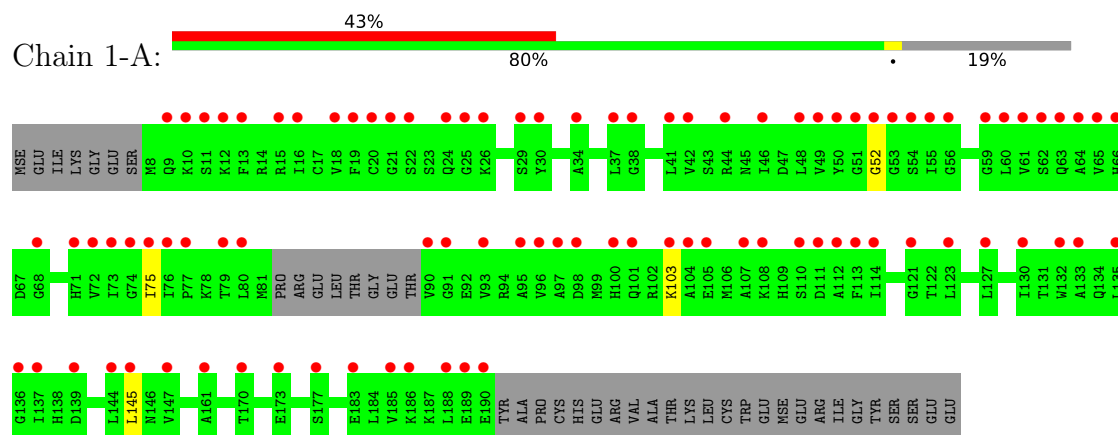
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	108	Total 108	O 108	0	0
4	1-B	114	Total 114	O 114	0	0

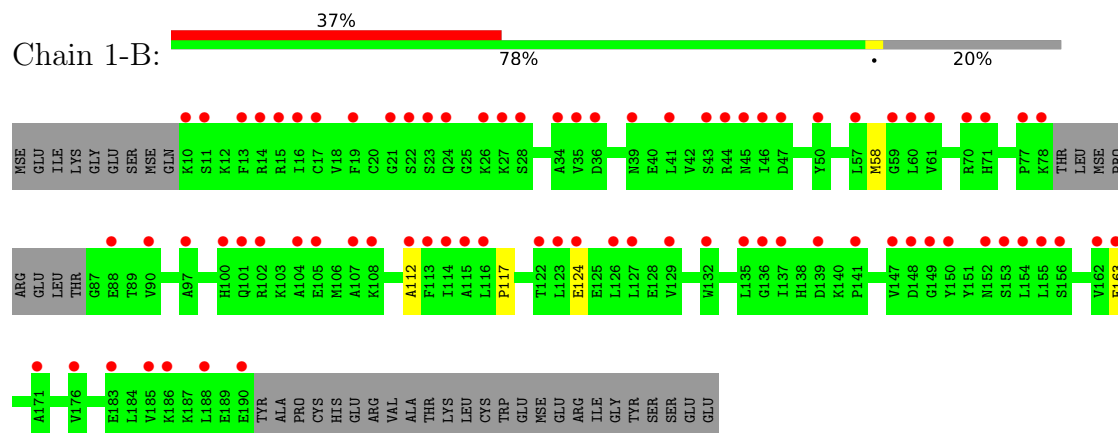
3 Residue-property plots

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.

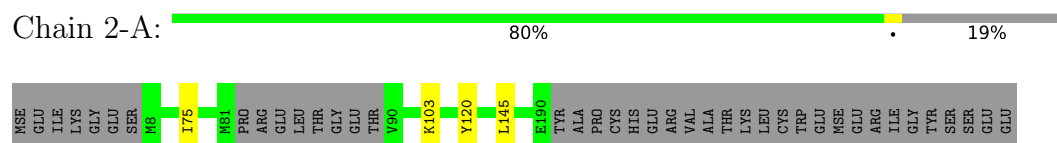
- Molecule 1: Uncharacterized protein At2g37210/T2N18.3



- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

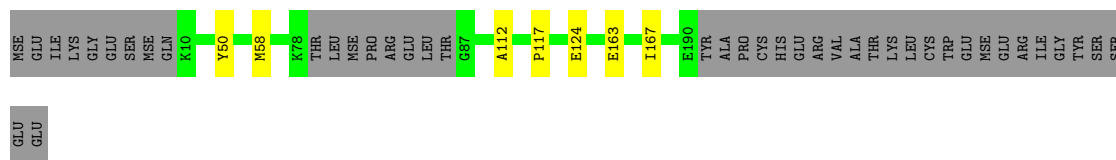


- Molecule 1: Uncharacterized protein At2g37210/T2N18.3



- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 2-B:  77% 20%



- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 3-A:  80% 19%



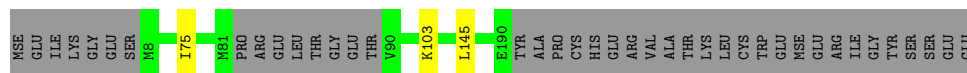
- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 3-B:  78% 20%



- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 4-A:  80% 19%



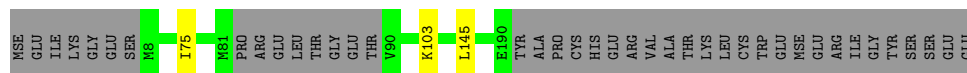
- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 4-B:  79% 20%



- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 5-A:  80% 19%



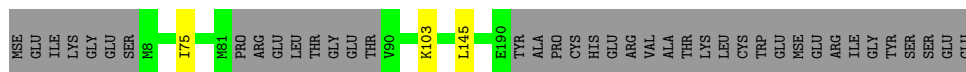
- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 5-B:  78% 20%



- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 6-A:  80% 19%



- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 6-B:  78% 20%



- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 7-A:  78% 19%



- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 7-B:  78% 20%



- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 8-A:  78% 19%



- Molecule 1: Uncharacterized protein At2g37210/T2N18.3

Chain 8-B:  79% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.40Å 66.77Å 98.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 1.95 46.96 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.96-1.95) 99.8 (46.96-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.168 , 0.224 0.182 , 0.231	Depositor DCC
R_{free} test set	1336 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.05 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	22875	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% 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: MG, 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	1-A	0.33	0/1344	0.44	0/1802
1	1-B	0.34	0/1325	0.44	0/1779
1	2-A	0.33	0/1344	0.44	0/1802
1	2-B	0.34	0/1325	0.44	0/1779
1	3-A	0.33	0/1344	0.44	0/1802
1	3-B	0.34	0/1325	0.44	0/1779
1	4-A	0.33	0/1344	0.44	0/1802
1	4-B	0.34	0/1325	0.44	0/1779
1	5-A	0.33	0/1344	0.44	0/1802
1	5-B	0.34	0/1325	0.44	0/1779
1	6-A	0.33	0/1344	0.44	0/1802
1	6-B	0.34	0/1325	0.44	0/1779
1	7-A	0.33	0/1344	0.44	0/1802
1	7-B	0.34	0/1325	0.44	0/1779
1	8-A	0.33	0/1344	0.44	0/1802
1	8-B	0.34	0/1325	0.44	0/1779
All	All	0.33	0/21352	0.44	0/28648

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	2-A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2-A	120	TYR	Sidechain

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	1-A	1328	0	1351	0	0
1	1-B	1308	0	1323	0	0
1	2-A	1328	0	1351	0	0
1	2-B	1308	0	1323	0	0
1	3-A	1328	0	1351	0	0
1	3-B	1308	0	1323	0	0
1	4-A	1328	0	1351	0	0
1	4-B	1308	0	1323	0	0
1	5-A	1328	0	1351	0	0
1	5-B	1308	0	1323	0	0
1	6-A	1328	0	1351	0	0
1	6-B	1308	0	1323	0	0
1	7-A	1328	0	1351	0	0
1	7-B	1308	0	1323	0	0
1	8-A	1328	0	1351	0	0
1	8-B	1308	0	1323	0	0
2	1-A	5	0	0	0	0
2	1-B	5	0	0	0	0
3	1-B	1	0	0	0	0
4	1-A	108	0	0	0	0
4	1-B	114	0	0	0	0
4	2-A	109	0	0	0	0
4	2-B	113	0	0	0	0
4	3-A	104	0	0	0	0
4	3-B	118	0	0	0	0
4	4-A	108	0	0	0	0
4	4-B	114	0	0	0	0
4	5-A	105	0	0	0	0
4	5-B	117	0	0	0	0
4	6-A	104	0	0	0	0
4	6-B	118	0	0	0	0
4	7-A	104	0	0	0	0
4	7-B	118	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	8-A	104	0	0	0	0
4	8-B	118	0	0	0	0
All	All	22875	0	21392	0	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 0.

There are no clashes within the asymmetric unit.

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	1-A	171/215 (80%)	164 (96%)	6 (4%)	1 (1%)	21	12
1	1-B	169/215 (79%)	165 (98%)	3 (2%)	1 (1%)	21	12
1	2-A	171/215 (80%)	163 (95%)	8 (5%)	0	100	100
1	2-B	169/215 (79%)	156 (92%)	10 (6%)	3 (2%)	6	1
1	3-A	171/215 (80%)	163 (95%)	7 (4%)	1 (1%)	21	12
1	3-B	169/215 (79%)	162 (96%)	6 (4%)	1 (1%)	21	12
1	4-A	171/215 (80%)	163 (95%)	8 (5%)	0	100	100
1	4-B	169/215 (79%)	163 (96%)	6 (4%)	0	100	100
1	5-A	171/215 (80%)	165 (96%)	6 (4%)	0	100	100
1	5-B	169/215 (79%)	162 (96%)	5 (3%)	2 (1%)	10	4
1	6-A	171/215 (80%)	164 (96%)	7 (4%)	0	100	100
1	6-B	169/215 (79%)	156 (92%)	11 (6%)	2 (1%)	10	4
1	7-A	171/215 (80%)	159 (93%)	7 (4%)	5 (3%)	3	0
1	7-B	169/215 (79%)	162 (96%)	6 (4%)	1 (1%)	21	12
1	8-A	171/215 (80%)	159 (93%)	8 (5%)	4 (2%)	5	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-B	169/215 (79%)	162 (96%)	7 (4%)	0	100	100
All	All	2720/3440 (79%)	2588 (95%)	111 (4%)	21 (1%)	16	8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	7-A	34	ALA
1	7-A	56	GLY
1	8-A	79	THR
1	8-A	97	ALA
1	2-B	112	ALA
1	3-B	96	VAL
1	6-B	189	GLU
1	7-A	128	GLU
1	8-A	80	LEU
1	2-B	50	TYR
1	7-A	103	LYS
1	1-A	52	GLY
1	1-B	112	ALA
1	2-B	167	ILE
1	7-B	148	ASP
1	8-A	121	GLY
1	5-B	65	VAL
1	6-B	137	ILE
1	7-A	35	VAL
1	3-A	96	VAL
1	5-B	77	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	1-A	142/170 (84%)	139 (98%)	3 (2%)	47	41
1	1-B	139/170 (82%)	135 (97%)	4 (3%)	37	29
1	2-A	142/170 (84%)	139 (98%)	3 (2%)	47	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2-B	139/170 (82%)	135 (97%)	4 (3%)	37	29
1	3-A	142/170 (84%)	139 (98%)	3 (2%)	47	41
1	3-B	139/170 (82%)	135 (97%)	4 (3%)	37	29
1	4-A	142/170 (84%)	139 (98%)	3 (2%)	47	41
1	4-B	139/170 (82%)	135 (97%)	4 (3%)	37	29
1	5-A	142/170 (84%)	139 (98%)	3 (2%)	47	41
1	5-B	139/170 (82%)	135 (97%)	4 (3%)	37	29
1	6-A	142/170 (84%)	139 (98%)	3 (2%)	47	41
1	6-B	139/170 (82%)	135 (97%)	4 (3%)	37	29
1	7-A	142/170 (84%)	139 (98%)	3 (2%)	47	41
1	7-B	139/170 (82%)	135 (97%)	4 (3%)	37	29
1	8-A	142/170 (84%)	139 (98%)	3 (2%)	47	41
1	8-B	139/170 (82%)	135 (97%)	4 (3%)	37	29
All	All	2248/2720 (83%)	2192 (98%)	56 (2%)	42	34

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	75	ILE
1	1-A	103	LYS
1	1-A	145	LEU
1	1-B	58	MSE
1	1-B	117	PRO
1	1-B	124	GLU
1	1-B	163	GLU
1	2-A	75	ILE
1	2-A	103	LYS
1	2-A	145	LEU
1	2-B	58	MSE
1	2-B	117	PRO
1	2-B	124	GLU
1	2-B	163	GLU
1	3-A	75	ILE
1	3-A	103	LYS
1	3-A	145	LEU
1	3-B	58	MSE
1	3-B	117	PRO

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Mol	Chain	Res	Type
1	3-B	124	GLU
1	3-B	163	GLU
1	4-A	75	ILE
1	4-A	103	LYS
1	4-A	145	LEU
1	4-B	58	MSE
1	4-B	117	PRO
1	4-B	124	GLU
1	4-B	163	GLU
1	5-A	75	ILE
1	5-A	103	LYS
1	5-A	145	LEU
1	5-B	58	MSE
1	5-B	117	PRO
1	5-B	124	GLU
1	5-B	163	GLU
1	6-A	75	ILE
1	6-A	103	LYS
1	6-A	145	LEU
1	6-B	58	MSE
1	6-B	117	PRO
1	6-B	124	GLU
1	6-B	163	GLU
1	7-A	75	ILE
1	7-A	103	LYS
1	7-A	145	LEU
1	7-B	58	MSE
1	7-B	117	PRO
1	7-B	124	GLU
1	7-B	163	GLU
1	8-A	75	ILE
1	8-A	103	LYS
1	8-A	145	LEU
1	8-B	58	MSE
1	8-B	117	PRO
1	8-B	124	GLU
1	8-B	163	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	9	GLN

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Mol	Chain	Res	Type
1	1-A	24	GLN
1	1-A	45	ASN
1	1-A	66	HIS
1	1-A	71	HIS
1	1-A	100	HIS
1	1-A	101	GLN
1	1-A	134	GLN
1	1-B	39	ASN
1	1-B	45	ASN
1	1-B	109	HIS
1	1-B	134	GLN
1	2-A	71	HIS
1	2-A	134	GLN
1	2-B	39	ASN
1	2-B	45	ASN
1	2-B	101	GLN
1	2-B	134	GLN
1	3-A	24	GLN
1	3-A	66	HIS
1	3-A	134	GLN
1	3-B	24	GLN
1	3-B	39	ASN
1	3-B	45	ASN
1	3-B	71	HIS
1	3-B	134	GLN
1	3-B	138	HIS
1	4-A	24	GLN
1	4-A	134	GLN
1	4-B	31	GLN
1	4-B	39	ASN
1	4-B	45	ASN
1	4-B	134	GLN
1	5-A	24	GLN
1	5-A	66	HIS
1	5-A	134	GLN
1	5-B	31	GLN
1	5-B	39	ASN
1	5-B	45	ASN
1	5-B	134	GLN
1	6-A	9	GLN
1	6-A	63	GLN
1	6-A	71	HIS

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Mol	Chain	Res	Type
1	6-A	109	HIS
1	6-A	134	GLN
1	6-B	39	ASN
1	7-A	24	GLN
1	7-A	63	GLN
1	7-A	109	HIS
1	7-A	134	GLN
1	7-B	39	ASN
1	7-B	45	ASN
1	7-B	66	HIS
1	8-A	100	HIS
1	8-A	109	HIS
1	8-A	134	GLN
1	8-B	39	ASN
1	8-B	45	ASN
1	8-B	101	GLN
1	8-B	134	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
2	SO4	1-A	600	-	4,4,4	0.47	0	6,6,6	0.73	0
2	SO4	1-B	500	-	4,4,4	0.80	0	6,6,6	0.63	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	1-A	170/215 (79%)	2.50	93 (54%)  	2, 3, 4, 8	170 (100%)
1	1-B	170/215 (79%)	2.20	79 (46%)  	1, 3, 4, 7	170 (100%)
1	2-A	0/215	-	-	-	-
1	2-B	0/215	-	-	-	-
1	3-A	0/215	-	-	-	-
1	3-B	0/215	-	-	-	-
1	4-A	0/215	-	-	-	-
1	4-B	0/215	-	-	-	-
1	5-A	0/215	-	-	-	-
1	5-B	0/215	-	-	-	-
1	6-A	0/215	-	-	-	-
1	6-B	0/215	-	-	-	-
1	7-A	0/215	-	-	-	-
1	7-B	0/215	-	-	-	-
1	8-A	0/215	-	-	-	-
1	8-B	0/215	-	-	-	-
All	All	340/3440 (9%)	2.35	172 (50%)  	1, 3, 4, 8	340 (100%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	51	GLY	9.1
1	1-A	91	GLY	8.6
1	1-B	113	PHE	8.3
1	1-A	52	GLY	7.3
1	1-A	10	LYS	6.8
1	1-A	93	VAL	6.6
1	1-A	49	VAL	6.5
1	1-A	80	LEU	6.5
1	1-B	155	LEU	6.5
1	1-A	9	GLN	6.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	71	HIS	6.0
1	1-A	114	ILE	5.7
1	1-A	21	GLY	5.4
1	1-B	114	ILE	5.3
1	1-A	19	PHE	5.2
1	1-A	20	CYS	5.2
1	1-B	107	ALA	5.2
1	1-B	112	ALA	5.2
1	1-A	90	VAL	5.1
1	1-B	162	VAL	5.1
1	1-A	11	SER	5.0
1	1-B	104	ALA	5.0
1	1-A	79	THR	5.0
1	1-A	95	ALA	4.9
1	1-B	147	VAL	4.7
1	1-B	149	GLY	4.6
1	1-A	50	TYR	4.5
1	1-B	10	LYS	4.4
1	1-A	30	TYR	4.4
1	1-A	53	GLY	4.4
1	1-A	72	VAL	4.4
1	1-B	60	LEU	4.3
1	1-B	137	ILE	4.3
1	1-A	74	GLY	4.3
1	1-A	63	GLN	4.2
1	1-B	108	LYS	4.0
1	1-B	123	LEU	4.0
1	1-A	101	GLN	3.9
1	1-B	101	GLN	3.9
1	1-B	100	HIS	3.9
1	1-B	154	LEU	3.9
1	1-A	103	LYS	3.9
1	1-B	57	LEU	3.8
1	1-B	46	ILE	3.8
1	1-A	12	LYS	3.8
1	1-B	148	ASP	3.8
1	1-A	24	GLN	3.7
1	1-A	144	LEU	3.7
1	1-A	190	GLU	3.7
1	1-B	78	LYS	3.7
1	1-B	129	VAL	3.6
1	1-A	147	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	64	ALA	3.5
1	1-A	18	VAL	3.4
1	1-B	19	PHE	3.4
1	1-B	44	ARG	3.4
1	1-A	137	ILE	3.4
1	1-A	113	PHE	3.4
1	1-A	41	LEU	3.4
1	1-B	14	ARG	3.4
1	1-B	122	THR	3.4
1	1-B	186	LYS	3.3
1	1-B	11	SER	3.3
1	1-A	188	LEU	3.3
1	1-B	41	LEU	3.3
1	1-A	22	SER	3.3
1	1-A	34	ALA	3.3
1	1-A	77	PRO	3.3
1	1-A	108	LYS	3.2
1	1-B	15	ARG	3.2
1	1-A	16	ILE	3.2
1	1-B	34	ALA	3.2
1	1-B	163	GLU	3.2
1	1-A	139	ASP	3.2
1	1-B	105	GLU	3.2
1	1-A	96	VAL	3.2
1	1-A	185	VAL	3.2
1	1-A	68	GLY	3.2
1	1-A	123	LEU	3.1
1	1-A	25	GLY	3.1
1	1-A	112	ALA	3.1
1	1-B	22	SER	3.1
1	1-B	17	CYS	3.1
1	1-B	77	PRO	3.1
1	1-B	115	ALA	3.1
1	1-A	135	LEU	3.0
1	1-B	27	LYS	3.0
1	1-A	130	ILE	3.0
1	1-B	188	LEU	3.0
1	1-A	55	ILE	3.0
1	1-A	62	SER	3.0
1	1-B	190	GLU	3.0
1	1-B	16	ILE	3.0
1	1-B	141	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	1-A	76	ILE	2.9
1	1-B	126	LEU	2.9
1	1-B	135	LEU	2.9
1	1-A	177	SER	2.9
1	1-B	185	VAL	2.9
1	1-B	43	SER	2.9
1	1-A	161	ALA	2.9
1	1-B	136	GLY	2.9
1	1-A	73	ILE	2.8
1	1-A	145	LEU	2.8
1	1-B	156	SER	2.8
1	1-A	61	VAL	2.8
1	1-B	127	LEU	2.8
1	1-A	98	ASP	2.8
1	1-B	90	VAL	2.8
1	1-B	171	ALA	2.7
1	1-A	183	GLU	2.7
1	1-A	60	LEU	2.7
1	1-A	127	LEU	2.7
1	1-A	75	ILE	2.7
1	1-A	132	TRP	2.7
1	1-B	13	PHE	2.7
1	1-A	66	HIS	2.7
1	1-B	97	ALA	2.7
1	1-B	183	GLU	2.7
1	1-B	36	ASP	2.6
1	1-B	132	TRP	2.6
1	1-B	102	ARG	2.6
1	1-B	24	GLN	2.6
1	1-B	88	GLU	2.6
1	1-B	61	VAL	2.6
1	1-B	124	GLU	2.6
1	1-B	35	VAL	2.6
1	1-B	150	TYR	2.5
1	1-A	111	ASP	2.5
1	1-A	37	LEU	2.5
1	1-A	29	SER	2.5
1	1-A	26	LYS	2.5
1	1-B	28	SER	2.5
1	1-B	153	SER	2.5
1	1-B	139	ASP	2.5
1	1-B	50	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	15	ARG	2.4
1	1-A	136	GLY	2.4
1	1-A	105	GLU	2.4
1	1-A	13	PHE	2.4
1	1-B	59	GLY	2.4
1	1-A	48	LEU	2.4
1	1-A	121	GLY	2.4
1	1-A	186	LYS	2.4
1	1-A	170	THR	2.3
1	1-B	45	ASN	2.3
1	1-A	44	ARG	2.3
1	1-A	56	GLY	2.3
1	1-A	46	ILE	2.3
1	1-A	189	GLU	2.3
1	1-B	21	GLY	2.2
1	1-B	176	VAL	2.2
1	1-B	26	LYS	2.2
1	1-B	70	ARG	2.2
1	1-A	54	SER	2.2
1	1-A	110	SER	2.2
1	1-A	104	ALA	2.2
1	1-B	152	ASN	2.2
1	1-B	71	HIS	2.2
1	1-A	107	ALA	2.2
1	1-B	47	ASP	2.1
1	1-B	116	LEU	2.1
1	1-A	133	ALA	2.1
1	1-A	42	VAL	2.1
1	1-A	100	HIS	2.1
1	1-A	65	VAL	2.1
1	1-B	39	ASN	2.1
1	1-A	38	GLY	2.0
1	1-A	59	GLY	2.0
1	1-A	97	ALA	2.0
1	1-A	173	GLU	2.0
1	1-B	23	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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($\text{\AA}^2$)	Q<0.9
3	MG	1-B	700	1/1	0.88	0.09	33,33,33,33	1
2	SO4	1-A	600	5/5	0.94	0.10	26,27,30,32	5
2	SO4	1-B	500	5/5	0.97	0.10	19,21,26,27	5

6.5 Other polymers [i](#)

There are no such residues in this entry.