



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:44 AM UTC

PDB ID : 7D8S / pdb_00007d8s
Title : MITF bHLHLZ apo structure
Authors : Guo, M.; Fang, P.; Wang, J.
Deposited on : 2020-10-09
Resolution : 2.28 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

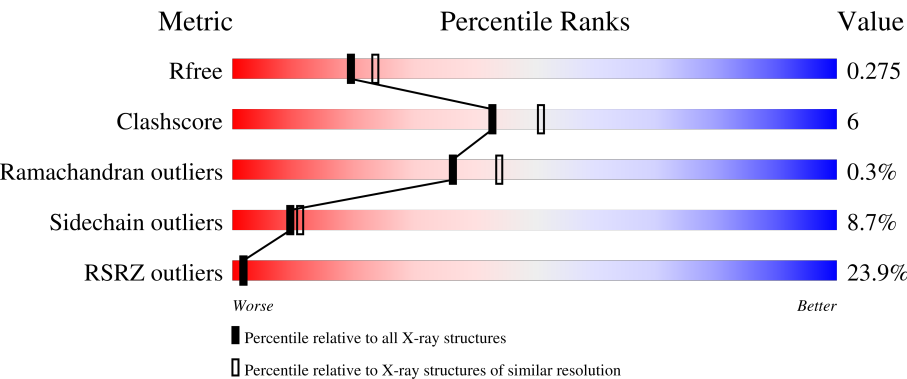
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	199	19% 75% 16% • 7%
1	B	199	24% 73% 13% 5% 10%
1	C	199	19% 78% 13% • 8%
1	D	199	26% 67% 18% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5762 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 Microphthalaria-associated transcription factor, Methionyl-tRNA synthetase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1382	882	243	254	3			
1	B	180	Total	C	N	O	S	0	0	0
			1329	847	239	241	2			
1	C	184	Total	C	N	O	S	0	0	0
			1411	894	253	262	2			
1	D	175	Total	C	N	O	S	0	0	0
			1313	836	230	244	3			

There are 24 discrepancies between the modelled and reference sequences:

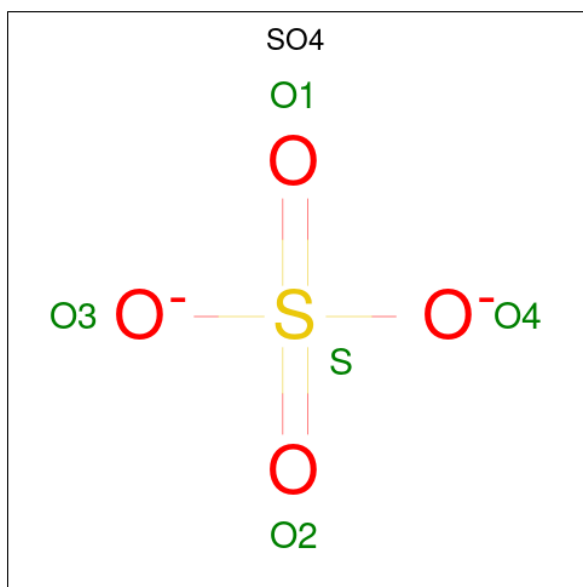
Chain	Residue	Modelled	Actual	Comment	Reference
A	305	SER	-	expression tag	UNP O75030
A	385	CYS	ASN	engineered mutation	UNP O75030
A	500	ALA	-	expression tag	UNP O66738
A	501	ALA	-	expression tag	UNP O66738
A	502	LEU	-	expression tag	UNP O66738
A	503	GLU	-	expression tag	UNP O66738
B	305	SER	-	expression tag	UNP O75030
B	385	CYS	ASN	engineered mutation	UNP O75030
B	500	ALA	-	expression tag	UNP O66738
B	501	ALA	-	expression tag	UNP O66738
B	502	LEU	-	expression tag	UNP O66738
B	503	GLU	-	expression tag	UNP O66738
C	305	SER	-	expression tag	UNP O75030
C	385	CYS	ASN	engineered mutation	UNP O75030
C	500	ALA	-	expression tag	UNP O66738
C	501	ALA	-	expression tag	UNP O66738
C	502	LEU	-	expression tag	UNP O66738
C	503	GLU	-	expression tag	UNP O66738
D	305	SER	-	expression tag	UNP O75030
D	385	CYS	ASN	engineered mutation	UNP O75030

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Chain	Residue	Modelled	Actual	Comment	Reference
D	500	ALA	-	expression tag	UNP O66738
D	501	ALA	-	expression tag	UNP O66738
D	502	LEU	-	expression tag	UNP O66738
D	503	GLU	-	expression tag	UNP O66738

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	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		

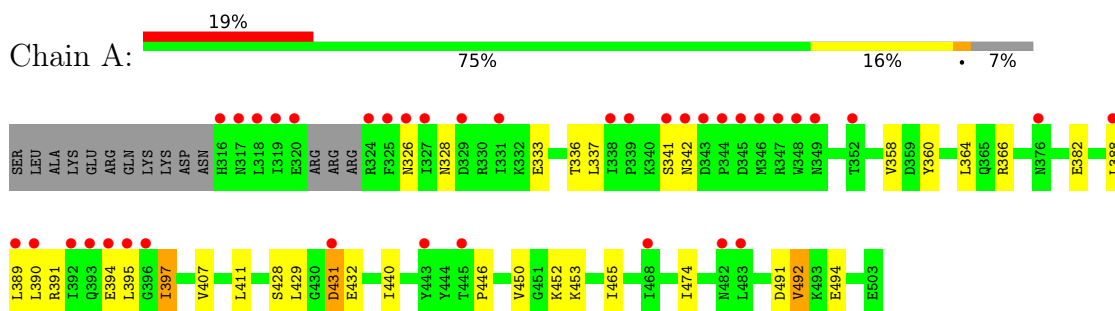
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total	O	0	0
			83	83		
3	B	72	Total	O	0	0
			72	72		
3	C	95	Total	O	0	0
			95	95		
3	D	62	Total	O	0	0
			62	62		

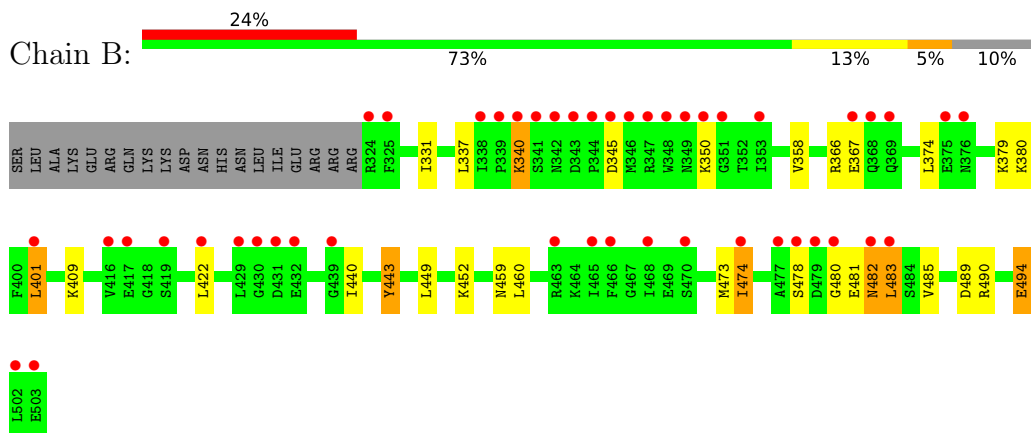
3 Residue-property plots

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.

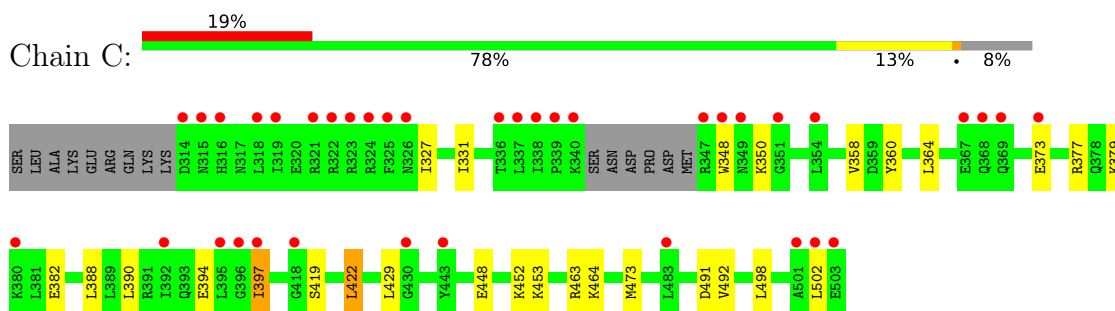
- Molecule 1: Microphthalmia-associated transcription factor,Methionyl-tRNA synthetase beta subunit



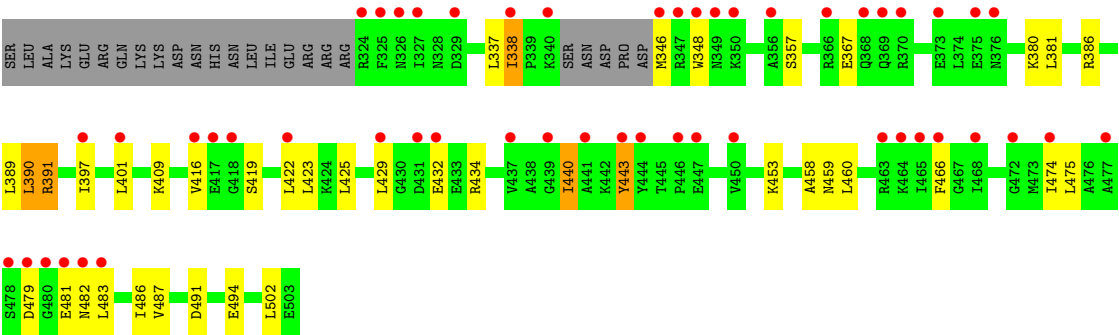
- Molecule 1: Microphthalmia-associated transcription factor,Methionyl-tRNA synthetase beta subunit



- Molecule 1: Microphthalmia-associated transcription factor,Methionyl-tRNA synthetase beta subunit



● Molecule 1: Microphthalmia-associated transcription factor,Methionyl-tRNA synthetase beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.01Å 62.31Å 65.31Å 90.12° 72.74° 86.39°	Depositor
Resolution (Å)	38.94 – 2.28 38.94 – 2.28	Depositor EDS
% Data completeness (in resolution range)	90.1 (38.94-2.28) 90.1 (38.94-2.28)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.25 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.231 , 0.271 0.235 , 0.275	Depositor DCC
R_{free} test set	1734 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5762	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.37	0/1395	0.79	2/1881 (0.1%)
1	B	0.47	0/1343	0.84	0/1817
1	C	0.39	0/1424	0.81	2/1916 (0.1%)
1	D	0.47	0/1324	0.89	4/1787 (0.2%)
All	All	0.42	0/5486	0.83	8/7401 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	458	ALA	N-CA-C	8.45	120.57	111.36
1	C	397	ILE	N-CA-C	7.77	118.82	111.91
1	D	429	LEU	N-CA-C	-6.21	105.46	113.16
1	D	459	ASN	N-CA-C	5.94	118.53	109.62
1	D	440	ILE	N-CA-C	5.63	118.40	112.83
1	C	429	LEU	N-CA-C	-5.50	106.34	113.16
1	A	397	ILE	N-CA-C	5.17	117.15	112.29
1	A	440	ILE	N-CA-C	5.04	117.82	112.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1382	0	1401	19	0
1	B	1329	0	1332	27	0
1	C	1411	0	1440	12	0
1	D	1313	0	1328	22	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	83	0	0	3	0
3	B	72	0	0	5	0
3	C	95	0	0	2	0
3	D	62	0	0	2	0
All	All	5762	0	5501	68	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 6.

All (68) 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:409:LYS:HB2	1:B:494:GLU:HG2	1.66	0.77
1:C:502:LEU:HA	3:C:716:HOH:O	1.88	0.74
1:C:358:VAL:HG13	1:D:337:LEU:HD11	1.76	0.67
1:B:391:ARG:CZ	1:D:380:LYS:HD3	2.25	0.67
1:D:409:LYS:HB2	1:D:494:GLU:HG2	1.76	0.66
1:B:482:ASN:HB2	3:B:739:HOH:O	1.98	0.63
1:C:463:ARG:HD2	3:C:787:HOH:O	1.97	0.63
1:D:416:VAL:HG11	1:D:422:LEU:HB2	1.81	0.63
1:D:453:LYS:NZ	1:D:491:ASP:OD1	2.32	0.62
1:B:497:LYS:NZ	3:B:705:HOH:O	2.32	0.62
1:A:328:ASN:ND2	3:A:603:HOH:O	2.30	0.61
1:B:482:ASN:CB	3:B:739:HOH:O	2.49	0.61
1:A:465:ILE:HD13	1:D:502:LEU:HD11	1.83	0.59
1:C:453:LYS:NZ	1:C:491:ASP:OD1	2.34	0.58
1:B:440:ILE:HG22	1:B:483:LEU:HD12	1.87	0.57
1:D:432:GLU:OE2	1:D:434:ARG:NE	2.35	0.56
1:B:443:TYR:CG	1:B:483:LEU:HB2	2.40	0.55
1:A:453:LYS:NZ	1:A:491:ASP:OD1	2.38	0.55
1:B:366:ARG:NE	3:B:704:HOH:O	2.31	0.53
1:B:490:ARG:NH2	1:C:448:GLU:OE2	2.41	0.53
1:B:473:MET:HG2	1:C:502:LEU:HD21	1.92	0.52
1:A:394:GLU:HB2	1:A:397:ILE:HD11	1.93	0.51
1:A:358:VAL:HG13	1:B:337:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:VAL:HG21	1:A:492:VAL:HG21	1.93	0.49
1:B:366:ARG:NH2	3:B:710:HOH:O	2.45	0.49
1:A:341:SER:O	1:A:342:ASN:CB	2.59	0.48
1:A:333:GLU:O	1:A:336:THR:OG1	2.21	0.48
1:A:391:ARG:O	1:A:394:GLU:HG2	2.12	0.48
1:A:366:ARG:NH2	3:A:607:HOH:O	2.40	0.48
1:C:331:ILE:HG21	1:C:350:LYS:HG2	1.94	0.48
1:A:411:LEU:HD11	1:A:428:SER:HB2	1.95	0.48
1:B:391:ARG:HB3	1:D:381:LEU:HD21	1.96	0.47
1:B:449:LEU:O	1:B:452:LYS:HB2	2.15	0.47
1:B:489:ASP:OD1	1:C:452:LYS:NZ	2.46	0.47
1:A:432:GLU:OE1	1:D:391:ARG:HD2	2.15	0.47
1:D:346:MET:HB3	1:D:348:TRP:CD1	2.51	0.46
1:D:367:GLU:O	3:D:702:HOH:O	2.21	0.46
1:B:478:SER:O	1:B:480:GLY:N	2.49	0.46
1:A:431:ASP:OD1	1:A:431:ASP:N	2.46	0.46
1:A:326:ASN:ND2	3:A:609:HOH:O	2.49	0.45
1:D:423:LEU:HD12	1:D:440:ILE:HG13	1.99	0.45
1:D:338:ILE:O	3:D:701:HOH:O	2.21	0.45
1:B:380:LYS:HD3	1:D:391:ARG:NH1	2.32	0.44
1:B:390:LEU:HD12	1:B:390:LEU:HA	1.81	0.43
1:B:331:ILE:HG21	1:B:350:LYS:HG2	1.99	0.43
1:D:416:VAL:HG13	1:D:419:SER:HB3	1.99	0.43
1:C:360:TYR:CE2	1:C:364:LEU:HD11	2.54	0.43
1:D:390:LEU:HD12	1:D:390:LEU:HA	1.80	0.42
1:D:475:LEU:HB3	1:D:486:ILE:HG13	2.01	0.42
1:B:459:ASN:O	1:B:460:LEU:HD12	2.19	0.42
1:B:494:GLU:CD	1:B:494:GLU:H	2.28	0.41
1:A:390:LEU:HD12	1:A:394:GLU:HG3	2.03	0.41
1:B:473:MET:HE3	1:B:473:MET:HB2	1.91	0.41
1:D:425:LEU:HD11	1:D:440:ILE:HD11	2.02	0.41
1:D:443:TYR:HE2	1:D:481:GLU:O	2.03	0.41
1:B:443:TYR:HE1	1:B:481:GLU:O	2.04	0.41
1:D:386:ARG:O	1:D:389:LEU:HB2	2.21	0.41
1:A:446:PRO:O	1:A:450:VAL:HG23	2.20	0.41
1:B:401:LEU:HD12	1:B:401:LEU:HA	1.87	0.40
1:D:409:LYS:CB	1:D:494:GLU:HG2	2.47	0.40
1:A:360:TYR:CE2	1:A:364:LEU:HD11	2.56	0.40
1:C:419:SER:OG	1:C:422:LEU:HB2	2.20	0.40
1:D:338:ILE:HD11	1:D:357:SER:N	2.37	0.40
1:A:337:LEU:HD11	1:B:358:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ILE:HD11	1:B:485:VAL:HG12	2.03	0.40
1:A:394:GLU:O	1:A:395:LEU:HD12	2.21	0.40
1:B:500:ALA:HB1	1:C:473:MET:HB2	2.03	0.40
1:C:394:GLU:O	1:C:397:ILE:HG12	2.22	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	181/199 (91%)	177 (98%)	4 (2%)	0	100	100
1	B	178/199 (89%)	172 (97%)	4 (2%)	2 (1%)	11	11
1	C	180/199 (90%)	177 (98%)	3 (2%)	0	100	100
1	D	171/199 (86%)	167 (98%)	4 (2%)	0	100	100
All	All	710/796 (89%)	693 (98%)	15 (2%)	2 (0%)	36	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	345	ASP
1	B	340	LYS

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	137/174 (79%)	128 (93%)	9 (7%)	15	19
1	B	128/174 (74%)	115 (90%)	13 (10%)	7	7
1	C	144/174 (83%)	132 (92%)	12 (8%)	10	12
1	D	130/174 (75%)	117 (90%)	13 (10%)	7	8
All	All	539/696 (77%)	492 (91%)	47 (9%)	9	11

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	GLU
1	A	388	LEU
1	A	389	LEU
1	A	429	LEU
1	A	431	ASP
1	A	452	LYS
1	A	474	ILE
1	A	492	VAL
1	A	494	GLU
1	B	340	LYS
1	B	367	GLU
1	B	374	LEU
1	B	379	LYS
1	B	390	LEU
1	B	391	ARG
1	B	401	LEU
1	B	422	LEU
1	B	443	TYR
1	B	474	ILE
1	B	482	ASN
1	B	483	LEU
1	B	494	GLU
1	C	327	ILE
1	C	348	TRP
1	C	373	GLU
1	C	377	ARG
1	C	379	LYS
1	C	382	GLU
1	C	388	LEU
1	C	390	LEU
1	C	422	LEU
1	C	464	LYS
1	C	492	VAL

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Mol	Chain	Res	Type
1	C	498	LEU
1	D	338	ILE
1	D	390	LEU
1	D	391	ARG
1	D	397	ILE
1	D	401	LEU
1	D	443	TYR
1	D	460	LEU
1	D	466	PHE
1	D	474	ILE
1	D	479	ASP
1	D	482	ASN
1	D	483	LEU
1	D	487	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	A	369	GLN
1	B	393	GLN
1	C	316	HIS
1	C	482	ASN
1	D	383	HIS
1	D	482	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	601	-	4,4,4	0.55	0	6,6,6	0.22	0
2	SO4	C	601	-	4,4,4	0.29	0	6,6,6	0.36	0
2	SO4	D	601	-	4,4,4	0.42	0	6,6,6	0.90	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	185/199 (92%)	1.41	38 (20%) 2 3	33, 52, 89, 118	0
1	B	180/199 (90%)	1.49	47 (26%) 1 1	32, 55, 91, 132	0
1	C	184/199 (92%)	1.18	37 (20%) 3 3	32, 50, 75, 92	0
1	D	175/199 (87%)	1.57	51 (29%) 1 1	32, 55, 76, 96	0
All	All	724/796 (90%)	1.41	173 (23%) 2 2	32, 54, 83, 132	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	ASP	5.5
1	A	392	ILE	5.3
1	A	316	HIS	4.9
1	B	347	ARG	4.8
1	A	348	TRP	4.8
1	B	478	SER	4.5
1	A	325	PHE	4.5
1	A	344	PRO	4.4
1	B	439	GLY	4.2
1	D	347	ARG	4.2
1	A	317	ASN	4.2
1	B	348	TRP	4.2
1	B	346	MET	4.1
1	A	345	ASP	4.1
1	B	480	GLY	4.1
1	C	337	LEU	4.0
1	A	396	GLY	4.0
1	B	479	ASP	4.0
1	A	346	MET	3.9
1	D	349	ASN	3.9
1	B	338	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	430	GLY	3.9
1	A	318	LEU	3.8
1	D	348	TRP	3.8
1	B	344	PRO	3.8
1	C	314	ASP	3.7
1	A	327	ILE	3.7
1	B	343	ASP	3.7
1	D	443	TYR	3.7
1	A	393	GLN	3.7
1	D	478	SER	3.7
1	B	466	PHE	3.6
1	D	474	ILE	3.6
1	A	342	ASN	3.6
1	B	430	GLY	3.6
1	B	422	LEU	3.5
1	C	348	TRP	3.5
1	A	326	ASN	3.4
1	D	431	ASP	3.4
1	B	341	SER	3.4
1	A	389	LEU	3.3
1	D	346	MET	3.3
1	D	422	LEU	3.3
1	C	340	LYS	3.3
1	D	368	GLN	3.3
1	A	320	GLU	3.2
1	C	392	ILE	3.2
1	D	416	VAL	3.2
1	B	502	LEU	3.2
1	D	464	LYS	3.1
1	A	394	GLU	3.1
1	B	342	ASN	3.1
1	C	418	GLY	3.1
1	B	465	ILE	3.0
1	D	338	ILE	3.0
1	D	441	ALA	3.0
1	C	318	LEU	3.0
1	A	338	ILE	3.0
1	C	319	ILE	3.0
1	A	347	ARG	3.0
1	C	323	ARG	3.0
1	B	482	ASN	3.0
1	A	395	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	373	GLU	3.0
1	C	321	ARG	2.9
1	A	319	ILE	2.9
1	B	340	LYS	2.9
1	B	483	LEU	2.9
1	D	480	GLY	2.8
1	D	437	VAL	2.8
1	B	339	PRO	2.8
1	D	417	GLU	2.8
1	D	350	LYS	2.8
1	A	390	LEU	2.7
1	D	439	GLY	2.7
1	A	339	PRO	2.7
1	D	329	ASP	2.7
1	A	443	TYR	2.6
1	B	345	ASP	2.6
1	C	396	GLY	2.6
1	A	341	SER	2.6
1	D	479	ASP	2.6
1	D	463	ARG	2.6
1	C	368	GLN	2.6
1	D	477	ALA	2.6
1	D	397	ILE	2.6
1	B	477	ALA	2.6
1	C	483	LEU	2.5
1	D	447	GLU	2.5
1	B	431	ASP	2.5
1	C	325	PHE	2.5
1	D	369	GLN	2.5
1	B	324	ARG	2.5
1	C	322	ARG	2.5
1	C	339	PRO	2.5
1	C	367	GLU	2.5
1	D	326	ASN	2.5
1	B	375	GLU	2.5
1	D	340	LYS	2.5
1	D	325	PHE	2.4
1	C	316	HIS	2.4
1	C	326	ASN	2.4
1	C	349	ASN	2.4
1	D	481	GLU	2.4
1	D	465	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	388	LEU	2.4
1	A	324	ARG	2.4
1	A	376	ASN	2.4
1	A	331	ILE	2.4
1	B	468	ILE	2.4
1	A	329	ASP	2.4
1	D	376	ASN	2.4
1	D	468	ILE	2.4
1	C	502	LEU	2.4
1	C	324	ARG	2.4
1	D	324	ARG	2.4
1	D	432	GLU	2.4
1	A	482	ASN	2.3
1	A	468	ILE	2.3
1	B	325	PHE	2.3
1	B	474	ILE	2.3
1	D	327	ILE	2.3
1	C	354	LEU	2.3
1	C	395	LEU	2.3
1	A	349	ASN	2.3
1	C	336	THR	2.3
1	C	338	ILE	2.3
1	B	349	ASN	2.3
1	B	350	LYS	2.3
1	C	315	ASN	2.3
1	D	472	GLY	2.3
1	B	463	ARG	2.3
1	B	503	GLU	2.3
1	C	397	ILE	2.3
1	A	483	LEU	2.2
1	D	450	VAL	2.3
1	D	466	PHE	2.2
1	B	368	GLN	2.2
1	B	419	SER	2.2
1	B	351	GLY	2.2
1	D	429	LEU	2.2
1	B	376	ASN	2.2
1	C	347	ARG	2.2
1	D	366	ARG	2.2
1	B	432	GLU	2.2
1	C	373	GLU	2.2
1	C	501	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	470	SER	2.2
1	B	353	ILE	2.2
1	D	370	ARG	2.2
1	B	416	VAL	2.2
1	C	380	LYS	2.2
1	D	356	ALA	2.2
1	D	444	TYR	2.1
1	B	401	LEU	2.1
1	B	429	LEU	2.1
1	D	482	ASN	2.1
1	B	417	GLU	2.1
1	A	445	THR	2.1
1	C	443	TYR	2.1
1	A	431	ASP	2.1
1	B	399	ASP	2.1
1	C	503	GLU	2.1
1	B	369	GLN	2.1
1	C	369	GLN	2.1
1	B	367	GLU	2.1
1	D	375	GLU	2.1
1	D	483	LEU	2.1
1	C	351	GLY	2.1
1	D	418	GLY	2.1
1	A	352	THR	2.0
1	D	401	LEU	2.0
1	D	446	PRO	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 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
2	SO4	D	601	5/5	0.83	0.16	77,77,77,77	0
2	SO4	C	601	5/5	0.86	0.13	86,86,86,87	0
2	SO4	B	601	5/5	0.96	0.09	62,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.