Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 04:10 PM JST

PDB ID	:	7D8S
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 (i) 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 (i)) were used in the production of this report:

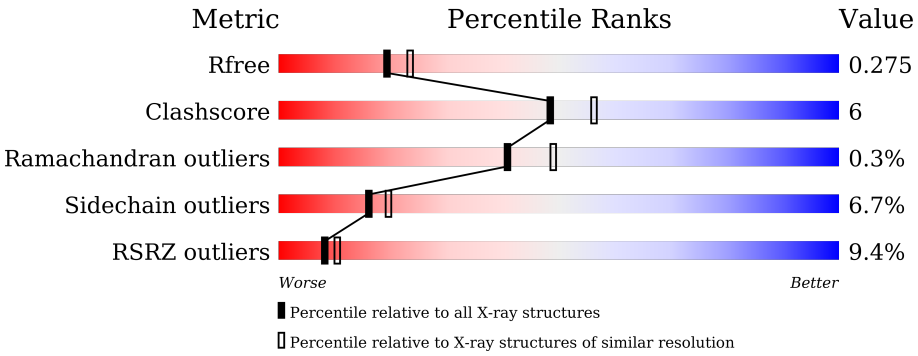
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (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 <=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	9% 77% 15% • 7%
1	B	199	13% 73% 14% • 10%
1	C	199	6% 81% 11% • 8%
1	D	199	7% 69% 17% • 12%

2 Entry composition (i)

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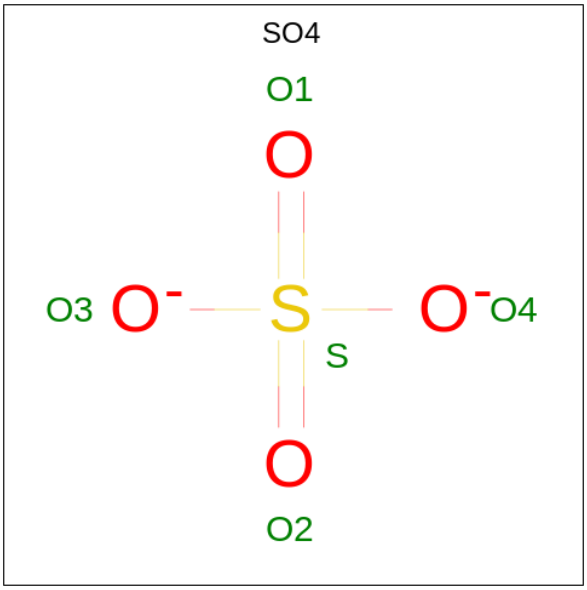
Chain	Residue	Modelled	Actual	Comment	Reference
D	500	ALA	-	expression tag	UNP O66738
D	501	ALA	-	expression tag	UNP O66738
D	502	LEU	-	expression tag	UNP O66738
D	503	GLU	-	expression tag	UNP O66738

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

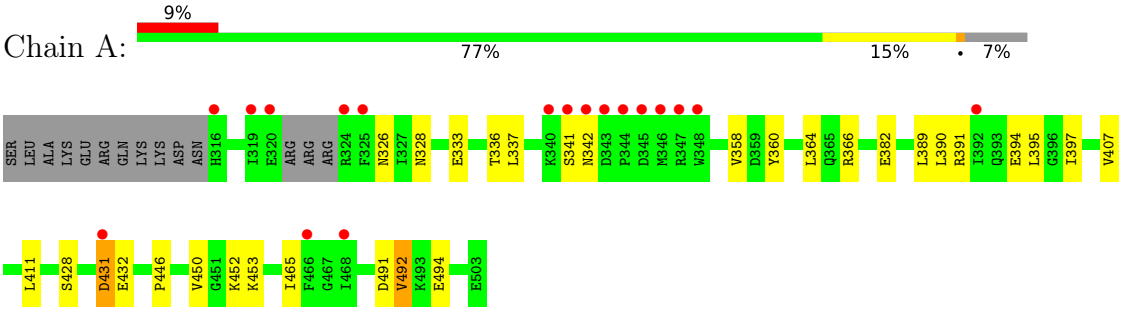
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	83	Total O 83 83	0	0
3	B	72	Total O 72 72	0	0
3	C	95	Total O 95 95	0	0
3	D	62	Total O 62 62	0	0

3 Residue-property plots (i)

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

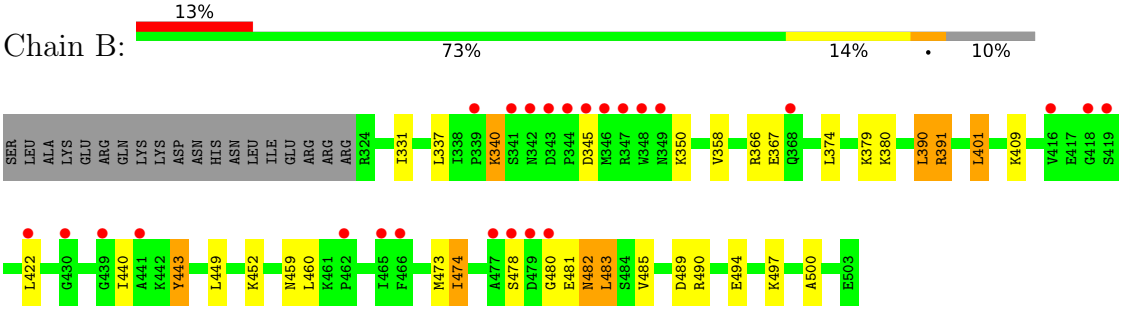
• Molecule 1: Microphthalmia-associated transcription factor,Methionyl-tRNA synthetase beta subunit

Chain A:



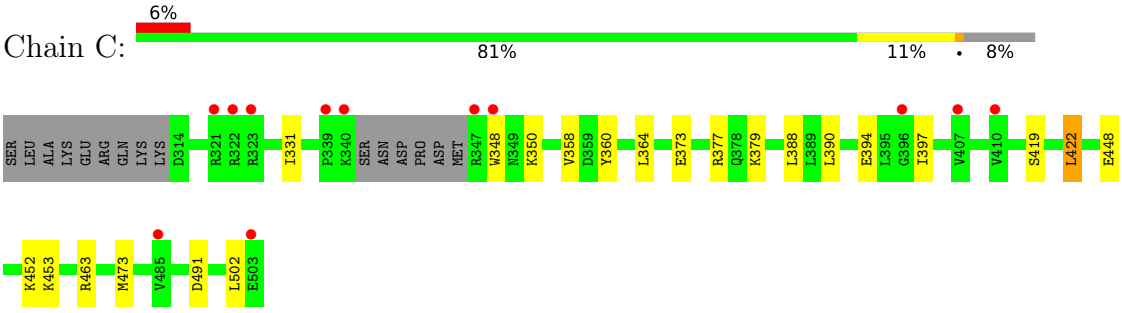
• Molecule 1: Microphthalmia-associated transcription factor,Methionyl-tRNA synthetase beta subunit

Chain B:



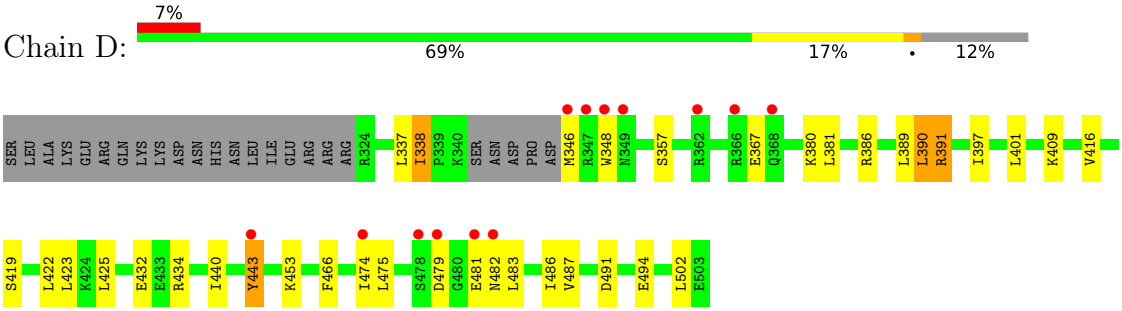
• Molecule 1: Microphthalmia-associated transcription factor,Methionyl-tRNA synthetase beta subunit

Chain C:



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

Chain D:


7%
69%
17%
12%
SER LEU ALA LYS GLU ARG GLN LYS LYS ASP ASN HIS ASN LEU ILE GLU ARG ARG ARG R324 L337 I338 P339 K340 SER ASN ASP PRO ASP M346 R347 W348 N349 S357 R362 R366 E367 Q368 K380 L381 R386 L389 L390 R391 I397 L401 K409 V416
S419 L422 L423 K424 L425 E432 E433 R434 I440 Y443 K453 F466 I474 L475 S478 D479 G480 E481 N482 L483 I486 V487 D491 E494 L502 E503

4 Data and refinement statistics (i)

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) 89.9 (38.94-2.28)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.25 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.231 , 0.271 0.234 , 0.275	Depositor DCC
R_{free} test set	1734 reflections (5.00%)	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)	0.31 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	0/1395	0.50	0/1881
1	B	0.34	0/1343	0.53	0/1817
1	C	0.32	0/1424	0.51	0/1916
1	D	0.35	0/1324	0.55	1/1787 (0.1%)
All	All	0.32	0/5486	0.52	1/7401 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	483	LEU	CA-CB-CG	5.53	128.03	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1382	0	1401	19	0
1	B	1329	0	1332	25	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	66	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 (66) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:390:LEU:HD12	1:A:394:GLU:HG3	2.03	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
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%)	14 14
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%)	41 49

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%)	131 (96%)	6 (4%)	28 37
1	B	128/174 (74%)	116 (91%)	12 (9%)	8 9
1	C	144/174 (83%)	137 (95%)	7 (5%)	25 33
1	D	130/174 (75%)	119 (92%)	11 (8%)	10 12
All	All	539/696 (77%)	503 (93%)	36 (7%)	16 19

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	GLU
1	A	389	LEU
1	A	431	ASP
1	A	452	LYS
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	C	348	TRP
1	C	373	GLU
1	C	377	ARG
1	C	379	LYS
1	C	388	LEU
1	C	390	LEU
1	C	422	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	466	PHE
1	D	474	ILE
1	D	479	ASP
1	D	482	ASN
1	D	487	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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 monosaccharides 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	0.61	0	6,6,6	0.23	0
2	SO4	C	601	-	4,4,4	0.26	0	6,6,6	0.37	0
2	SO4	D	601	-	4,4,4	0.41	0	6,6,6	0.97	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	185/199 (92%)	0.72	18 (9%) 7 10	33, 52, 89, 118	0
1	B	180/199 (90%)	0.98	25 (13%) 2 3	32, 55, 91, 132	0
1	C	184/199 (92%)	0.74	12 (6%) 18 23	32, 50, 75, 92	0
1	D	175/199 (87%)	0.81	13 (7%) 14 18	32, 55, 76, 96	0
All	All	724/796 (90%)	0.81	68 (9%) 8 10	32, 54, 83, 132	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	ASP	6.7
1	B	344	PRO	6.7
1	B	466	PHE	6.4
1	C	348	TRP	6.3
1	A	325	PHE	6.2
1	A	346	MET	5.4
1	B	345	ASP	5.4
1	B	347	ARG	5.3
1	B	341	SER	5.3
1	A	344	PRO	5.1
1	A	341	SER	5.1
1	B	346	MET	4.7
1	B	465	ILE	4.7
1	B	342	ASN	4.7
1	C	321	ARG	4.4
1	A	392	ILE	4.1
1	A	348	TRP	3.7
1	B	416	VAL	3.6
1	D	346	MET	3.5
1	D	368	GLN	3.5
1	B	430	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	396	GLY	3.3
1	A	316	HIS	3.3
1	C	339	PRO	3.2
1	D	443	TYR	3.2
1	D	348	TRP	3.2
1	D	479	ASP	3.2
1	D	478	SER	3.1
1	C	347	ARG	3.1
1	D	366	ARG	3.1
1	D	347	ARG	3.1
1	A	342	ASN	3.0
1	A	343	ASP	3.0
1	C	340	LYS	3.0
1	B	478	SER	3.0
1	B	480	GLY	2.9
1	C	503	GLU	2.9
1	A	345	ASP	2.9
1	A	340	LYS	2.8
1	D	482	ASN	2.8
1	B	462	PRO	2.8
1	C	407	VAL	2.6
1	A	319	ILE	2.6
1	B	439	GLY	2.5
1	B	479	ASP	2.5
1	C	322	ARG	2.3
1	C	485	VAL	2.3
1	A	324	ARG	2.3
1	B	368	GLN	2.3
1	B	419	SER	2.3
1	A	347	ARG	2.2
1	D	481	GLU	2.2
1	B	477	ALA	2.2
1	C	410	VAL	2.2
1	D	349	ASN	2.2
1	A	466	PHE	2.2
1	A	431	ASP	2.2
1	D	362	ARG	2.1
1	D	474	ILE	2.1
1	B	422	LEU	2.1
1	B	418	GLY	2.1
1	A	320	GLU	2.1
1	C	323	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	349	ASN	2.1
1	A	468	ILE	2.1
1	B	339	PRO	2.1
1	B	348	TRP	2.0
1	B	441	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	601	5/5	0.92	0.16	77,77,77,77	0
2	SO4	C	601	5/5	0.94	0.12	86,86,86,87	0
2	SO4	B	601	5/5	0.96	0.13	62,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.