



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 07:33 PM BST

PDB ID : 5ZNY
Title : Structure of mDR3_DD-C363G with MBP tag
Authors : Yin, X.; Jin, T.
Deposited on : 2018-04-11
Resolution : 2.74 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

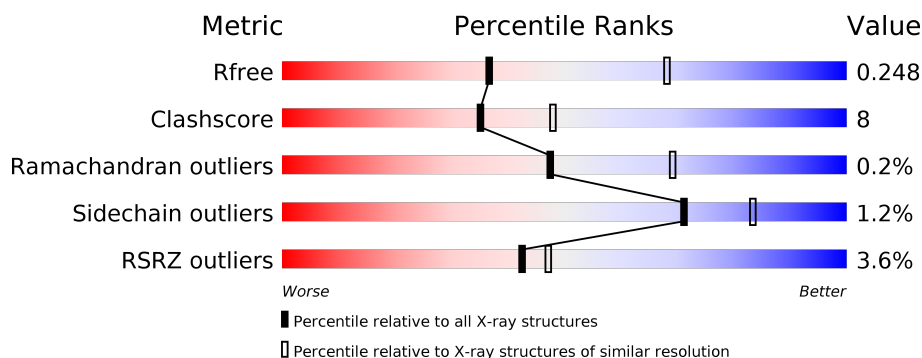
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 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	464	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div></div> </div> <div></div> </div>
1	B	464	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div></div> </div> <div></div> </div>
1	C	464	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div></div> </div> <div></div> </div>
1	D	464	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div></div> </div> <div></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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	D	505	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14098 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 Maltose-binding periplasmic protein,Tumor necrosis factor receptor superfamily, member 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3470	2225	579	656	10			
1	B	450	Total	C	N	O	S	0	0	0
			3487	2234	584	659	10			
1	C	450	Total	C	N	O	S	0	0	0
			3487	2234	584	659	10			
1	D	453	Total	C	N	O	S	0	0	0
			3515	2252	591	662	10			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P0AEX9
A	83	ALA	ASP	engineered mutation	UNP P0AEX9
A	84	ALA	LYS	engineered mutation	UNP P0AEX9
A	173	ALA	GLU	engineered mutation	UNP P0AEX9
A	174	ALA	ASN	engineered mutation	UNP P0AEX9
A	240	ALA	LYS	engineered mutation	UNP P0AEX9
A	360	ALA	GLU	engineered mutation	UNP P0AEX9
A	363	ALA	LYS	engineered mutation	UNP P0AEX9
A	364	ALA	ASP	engineered mutation	UNP P0AEX9
A	368	ASN	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	371	ARG	-	linker	UNP P0AEX9
A	372	ALA	-	linker	UNP P0AEX9
A	373	ALA	-	linker	UNP P0AEX9
A	374	ALA	-	linker	UNP P0AEX9
A	410	GLY	CYS	engineered mutation	UNP B1AWN9
A	457	LEU	-	expression tag	UNP B1AWN9
A	458	GLU	-	expression tag	UNP B1AWN9
A	459	HIS	-	expression tag	UNP B1AWN9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	HIS	-	expression tag	UNP B1AWN9
A	461	HIS	-	expression tag	UNP B1AWN9
A	462	HIS	-	expression tag	UNP B1AWN9
A	463	HIS	-	expression tag	UNP B1AWN9
A	464	HIS	-	expression tag	UNP B1AWN9
B	1	MET	-	expression tag	UNP P0AEX9
B	83	ALA	ASP	engineered mutation	UNP P0AEX9
B	84	ALA	LYS	engineered mutation	UNP P0AEX9
B	173	ALA	GLU	engineered mutation	UNP P0AEX9
B	174	ALA	ASN	engineered mutation	UNP P0AEX9
B	240	ALA	LYS	engineered mutation	UNP P0AEX9
B	360	ALA	GLU	engineered mutation	UNP P0AEX9
B	363	ALA	LYS	engineered mutation	UNP P0AEX9
B	364	ALA	ASP	engineered mutation	UNP P0AEX9
B	368	ASN	-	linker	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
B	371	ARG	-	linker	UNP P0AEX9
B	372	ALA	-	linker	UNP P0AEX9
B	373	ALA	-	linker	UNP P0AEX9
B	374	ALA	-	linker	UNP P0AEX9
B	410	GLY	CYS	engineered mutation	UNP B1AWN9
B	457	LEU	-	expression tag	UNP B1AWN9
B	458	GLU	-	expression tag	UNP B1AWN9
B	459	HIS	-	expression tag	UNP B1AWN9
B	460	HIS	-	expression tag	UNP B1AWN9
B	461	HIS	-	expression tag	UNP B1AWN9
B	462	HIS	-	expression tag	UNP B1AWN9
B	463	HIS	-	expression tag	UNP B1AWN9
B	464	HIS	-	expression tag	UNP B1AWN9
C	1	MET	-	expression tag	UNP P0AEX9
C	83	ALA	ASP	engineered mutation	UNP P0AEX9
C	84	ALA	LYS	engineered mutation	UNP P0AEX9
C	173	ALA	GLU	engineered mutation	UNP P0AEX9
C	174	ALA	ASN	engineered mutation	UNP P0AEX9
C	240	ALA	LYS	engineered mutation	UNP P0AEX9
C	360	ALA	GLU	engineered mutation	UNP P0AEX9
C	363	ALA	LYS	engineered mutation	UNP P0AEX9
C	364	ALA	ASP	engineered mutation	UNP P0AEX9
C	368	ASN	-	linker	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
C	370	ALA	-	linker	UNP P0AEX9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	371	ARG	-	linker	UNP P0AEX9
C	372	ALA	-	linker	UNP P0AEX9
C	373	ALA	-	linker	UNP P0AEX9
C	374	ALA	-	linker	UNP P0AEX9
C	410	GLY	CYS	engineered mutation	UNP B1AWN9
C	457	LEU	-	expression tag	UNP B1AWN9
C	458	GLU	-	expression tag	UNP B1AWN9
C	459	HIS	-	expression tag	UNP B1AWN9
C	460	HIS	-	expression tag	UNP B1AWN9
C	461	HIS	-	expression tag	UNP B1AWN9
C	462	HIS	-	expression tag	UNP B1AWN9
C	463	HIS	-	expression tag	UNP B1AWN9
C	464	HIS	-	expression tag	UNP B1AWN9
D	1	MET	-	expression tag	UNP P0AEX9
D	83	ALA	ASP	engineered mutation	UNP P0AEX9
D	84	ALA	LYS	engineered mutation	UNP P0AEX9
D	173	ALA	GLU	engineered mutation	UNP P0AEX9
D	174	ALA	ASN	engineered mutation	UNP P0AEX9
D	240	ALA	LYS	engineered mutation	UNP P0AEX9
D	360	ALA	GLU	engineered mutation	UNP P0AEX9
D	363	ALA	LYS	engineered mutation	UNP P0AEX9
D	364	ALA	ASP	engineered mutation	UNP P0AEX9
D	368	ASN	-	linker	UNP P0AEX9
D	369	ALA	-	linker	UNP P0AEX9
D	370	ALA	-	linker	UNP P0AEX9
D	371	ARG	-	linker	UNP P0AEX9
D	372	ALA	-	linker	UNP P0AEX9
D	373	ALA	-	linker	UNP P0AEX9
D	374	ALA	-	linker	UNP P0AEX9
D	410	GLY	CYS	engineered mutation	UNP B1AWN9
D	457	LEU	-	expression tag	UNP B1AWN9
D	458	GLU	-	expression tag	UNP B1AWN9
D	459	HIS	-	expression tag	UNP B1AWN9
D	460	HIS	-	expression tag	UNP B1AWN9
D	461	HIS	-	expression tag	UNP B1AWN9
D	462	HIS	-	expression tag	UNP B1AWN9
D	463	HIS	-	expression tag	UNP B1AWN9
D	464	HIS	-	expression tag	UNP B1AWN9

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



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

Continued on next page...

Continued from previous page...

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	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	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	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

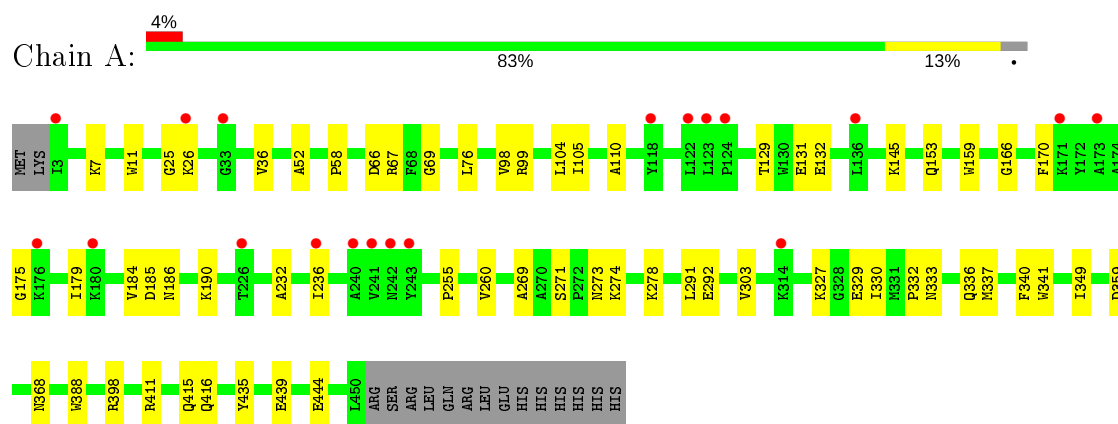
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	2	Total	O	0	0
			2	2		
3	C	1	Total	O	0	0
			1	1		

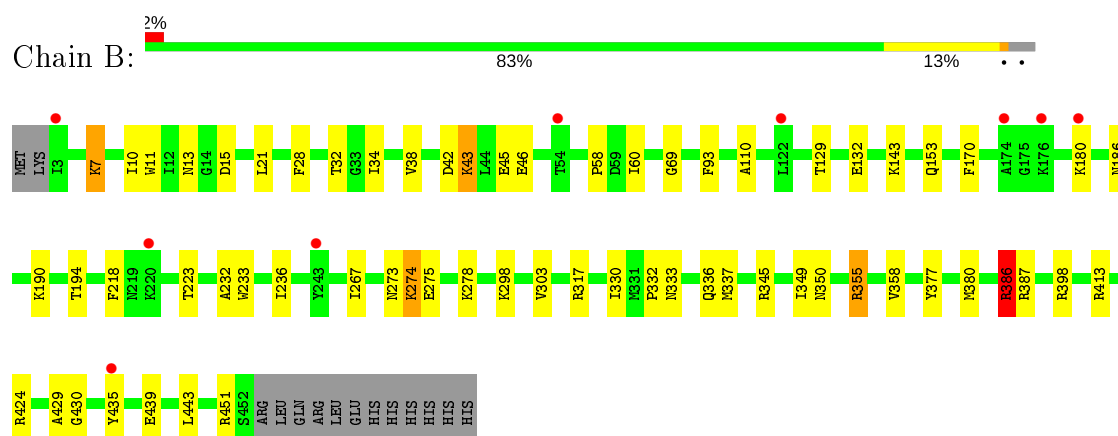
3 Residue-property plots [i](#)

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.

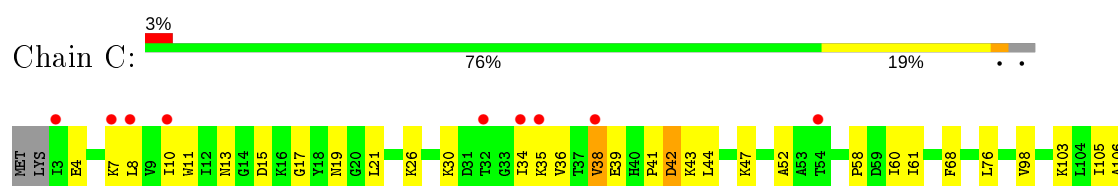
- Molecule 1: Maltose-binding periplasmic protein,Tumor necrosis factor receptor superfamily, member 25

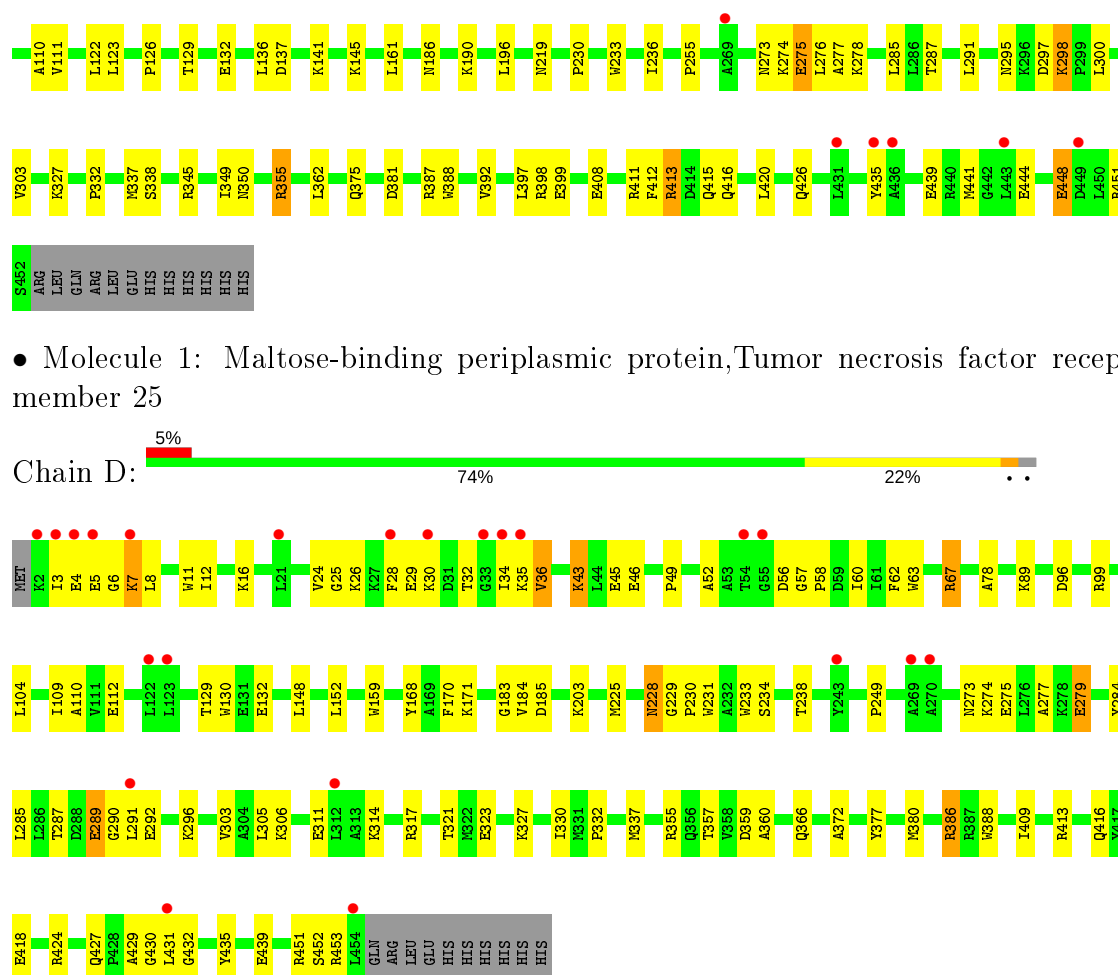


- Molecule 1: Maltose-binding periplasmic protein,Tumor necrosis factor receptor superfamily, member 25



- Molecule 1: Maltose-binding periplasmic protein,Tumor necrosis factor receptor superfamily, member 25





- Molecule 1: Maltose-binding periplasmic protein,Tumor necrosis factor receptor superfamily, member 25

Chain D: 5% 74% 22% . .

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.32Å 145.15Å 178.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.78 – 2.74 47.78 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.78-2.74) 99.7 (47.78-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, R_{free}	0.210 , 0.248 0.210 , 0.248	Depositor DCC
R_{free} test set	3109 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.6	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	0.95	EDS
Total number of atoms	14098	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3250e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 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	0.43	1/3550 (0.0%)	0.62	4/4819 (0.1%)
1	B	0.45	1/3567 (0.0%)	0.83	16/4841 (0.3%)
1	C	0.45	0/3567	0.76	12/4841 (0.2%)
1	D	0.53	6/3595 (0.2%)	0.86	19/4877 (0.4%)
All	All	0.47	8/14279 (0.1%)	0.77	51/19378 (0.3%)

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	B	0	1
1	D	0	1
All	All	0	2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4	GLU	CB-CG	8.04	1.67	1.52
1	D	289	GLU	CB-CG	-7.07	1.38	1.52
1	B	180	LYS	CD-CE	6.65	1.67	1.51
1	D	4	GLU	CD-OE2	6.41	1.32	1.25
1	D	289	GLU	CG-CD	-6.19	1.42	1.51

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ARG	NE-CZ-NH2	-20.45	110.07	120.30
1	D	386	ARG	NE-CZ-NH2	-15.31	112.64	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	355	ARG	CB-CG-CD	-14.63	73.56	111.60
1	B	386	ARG	NE-CZ-NH1	14.22	127.41	120.30
1	D	386	ARG	CD-NE-CZ	11.55	139.77	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	386	ARG	Sidechain
1	D	386	ARG	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	A	3470	0	3432	42	0
1	B	3487	0	3449	39	0
1	C	3487	0	3450	68	0
1	D	3515	0	3486	81	0
2	A	25	0	0	1	0
2	B	35	0	0	0	0
2	C	35	0	0	1	0
2	D	40	0	0	3	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	14098	0	13817	229	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 8.

The worst 5 of 229 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:10:ILE:HD11	1:B:38:VAL:HG22	1.41	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:LYS:HA	1:D:34:ILE:HD11	1.45	0.96
1:D:275:GLU:OE2	1:D:279:GLU:HG3	1.67	0.93
1:D:228:ASN:HD22	1:D:229:GLY:H	1.06	0.93
1:D:24:VAL:HG11	1:D:290:GLY:HA2	1.56	0.88

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	446/464 (96%)	431 (97%)	14 (3%)	1 (0%)	47	69
1	B	448/464 (97%)	439 (98%)	9 (2%)	0	100	100
1	C	448/464 (97%)	438 (98%)	9 (2%)	1 (0%)	47	69
1	D	451/464 (97%)	440 (98%)	10 (2%)	1 (0%)	47	69
All	All	1793/1856 (97%)	1748 (98%)	42 (2%)	3 (0%)	47	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	448	GLU
1	D	452	SER
1	A	175	GLY

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	347/363 (96%)	345 (99%)	2 (1%)	86	91
1	B	349/363 (96%)	345 (99%)	4 (1%)	73	84
1	C	349/363 (96%)	344 (99%)	5 (1%)	67	80
1	D	352/363 (97%)	346 (98%)	6 (2%)	60	76
All	All	1397/1452 (96%)	1380 (99%)	17 (1%)	71	83

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	285	LEU
1	C	298	LYS
1	D	171	LYS
1	C	26	LYS
1	D	228	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	GLN
1	D	326	GLN
1	C	375	GLN
1	A	425	GLN
1	C	295	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

27 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	D	505	1	4,4,4	0.39	0	6,6,6	0.28	0
2	SO4	D	502	-	4,4,4	0.36	0	6,6,6	0.64	0
2	SO4	D	506	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	C	507	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	B	507	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	C	502	-	4,4,4	0.12	0	6,6,6	0.09	0
2	SO4	B	501	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	C	505	-	4,4,4	0.15	0	6,6,6	0.22	0
2	SO4	B	502	-	4,4,4	0.13	0	6,6,6	0.04	0
2	SO4	B	505	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	D	507	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	C	503	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	B	503	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	A	502	-	4,4,4	0.12	0	6,6,6	0.09	0
2	SO4	A	505	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	A	504	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	A	503	-	4,4,4	0.13	0	6,6,6	0.40	0
2	SO4	D	508	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	A	501	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	C	501	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SO4	B	506	1	4,4,4	0.25	0	6,6,6	0.38	0
2	SO4	C	504	-	4,4,4	0.10	0	6,6,6	0.34	0
2	SO4	B	504	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	D	504	-	4,4,4	0.17	0	6,6,6	0.07	0
2	SO4	D	503	-	4,4,4	0.13	0	6,6,6	0.05	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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	505	SO4	2	0
2	C	505	SO4	1	0
2	A	504	SO4	1	0
2	D	503	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	448/464 (96%)	0.36	19 (4%) 36 39	50, 75, 110, 155	0
1	B	450/464 (96%)	0.28	9 (2%) 65 72	49, 73, 108, 153	0
1	C	450/464 (96%)	0.38	15 (3%) 46 52	49, 76, 123, 159	0
1	D	453/464 (97%)	0.50	22 (4%) 29 33	44, 83, 129, 158	0
All	All	1801/1856 (97%)	0.38	65 (3%) 42 47	44, 76, 118, 159	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	431	LEU	6.7
1	D	3	ILE	5.6
1	D	270	ALA	5.1
1	C	54	THR	4.6
1	A	180	LYS	4.4

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, 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(\AA^2)	Q<0.9
2	SO4	A	505	5/5	0.74	0.33	166,168,168,168	0
2	SO4	D	505	5/5	0.79	0.19	116,117,117,119	0
2	SO4	D	508	5/5	0.79	0.28	157,157,158,158	0
2	SO4	B	504	5/5	0.82	0.28	133,134,135,135	0
2	SO4	D	506	5/5	0.83	0.23	142,144,145,145	0
2	SO4	B	502	5/5	0.84	0.30	163,163,164,165	0
2	SO4	C	506	5/5	0.85	0.20	136,137,138,138	0
2	SO4	C	502	5/5	0.85	0.24	128,128,128,129	0
2	SO4	C	501	5/5	0.86	0.18	127,129,130,130	0
2	SO4	D	507	5/5	0.88	0.20	151,151,151,152	0
2	SO4	C	503	5/5	0.89	0.12	162,162,163,163	0
2	SO4	D	501	5/5	0.89	0.15	132,133,134,134	0
2	SO4	B	507	5/5	0.90	0.20	146,146,147,147	0
2	SO4	D	504	5/5	0.90	0.17	131,131,131,133	0
2	SO4	A	501	5/5	0.91	0.16	124,125,125,125	0
2	SO4	B	501	5/5	0.91	0.13	117,119,120,120	0
2	SO4	C	507	5/5	0.93	0.25	150,150,150,152	0
2	SO4	B	506	5/5	0.93	0.24	88,89,91,93	0
2	SO4	B	505	5/5	0.94	0.19	113,113,114,114	0
2	SO4	D	503	5/5	0.94	0.15	103,104,105,106	0
2	SO4	A	502	5/5	0.95	0.17	132,132,133,133	0
2	SO4	C	505	5/5	0.98	0.13	69,71,73,74	0
2	SO4	C	504	5/5	0.98	0.15	69,69,71,72	0
2	SO4	B	503	5/5	0.98	0.17	67,68,71,73	0
2	SO4	A	504	5/5	0.98	0.16	69,70,71,78	0
2	SO4	A	503	5/5	0.98	0.16	69,71,72,78	0
2	SO4	D	502	5/5	0.99	0.25	67,69,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.