



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 10:21 PM EDT

PDB ID : 5I82  
Title : First Crystal Structure of E.coli Based Recombinant Diphtheria Toxin Mutant CRM197  
Authors : Minasov, G.; Shuvalova, L.; Mishra, R.P.N.; Goel, A.; Dubrovskaya, I.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2016-02-18  
Resolution : 2.35 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](mailto: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>.

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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 : 2.35.1  
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

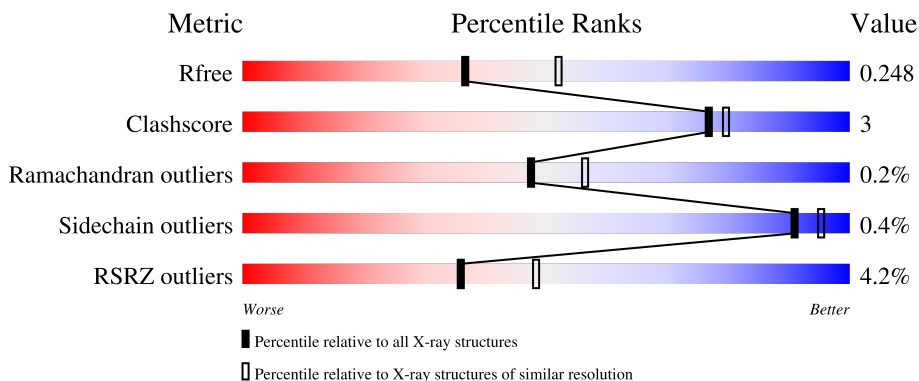
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\geq 3$ , 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	535	 4% 88% 7% 5%
1	B	535	 4% 86% 9% 5%
1	C	535	 4% 90% 6% .
1	D	535	 4% 89% 6% 5%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16104 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 Diphtheria toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	509	3915	2468	665	770	12	0	0	0
1	B	510	3935	2481	667	775	12	0	0	0
1	C	514	3959	2495	671	781	12	0	0	0
1	D	507	3921	2471	667	771	12	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	GLU	GLY	engineered mutation	UNP Q5PY51
B	52	GLU	GLY	engineered mutation	UNP Q5PY51
C	52	GLU	GLY	engineered mutation	UNP Q5PY51
D	52	GLU	GLY	engineered mutation	UNP Q5PY51

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

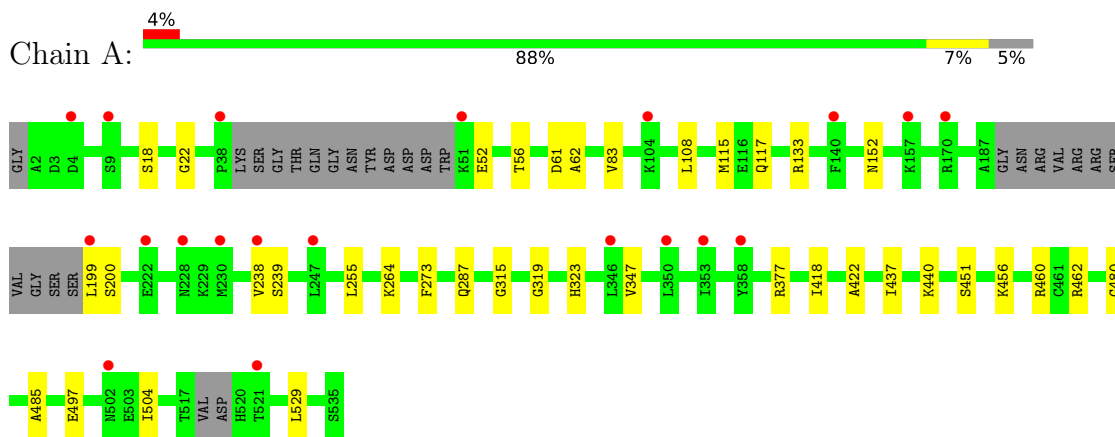
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	94	Total 94	O 94	0	0
4	B	88	Total 88	O 88	0	0
4	C	90	Total 91	O 91	0	1
4	D	79	Total 80	O 80	0	2

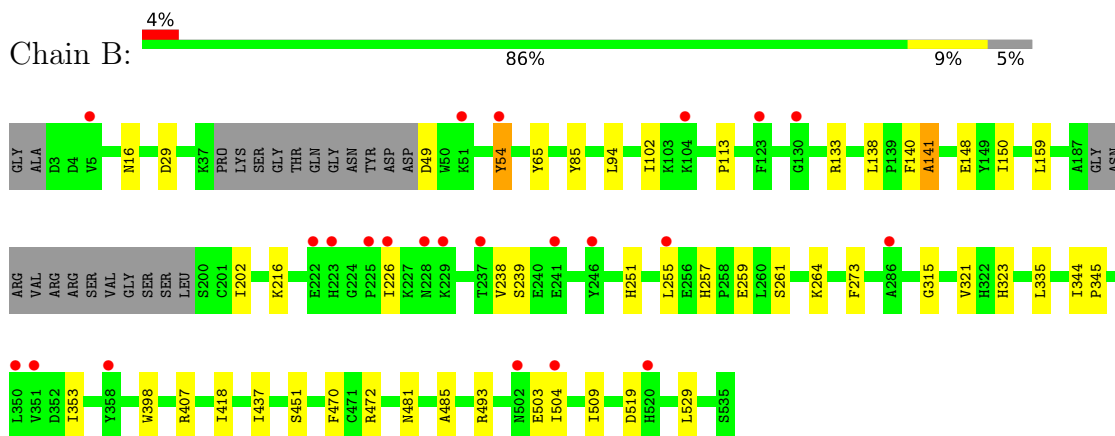
### 3 Residue-property plots [i](#)

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.

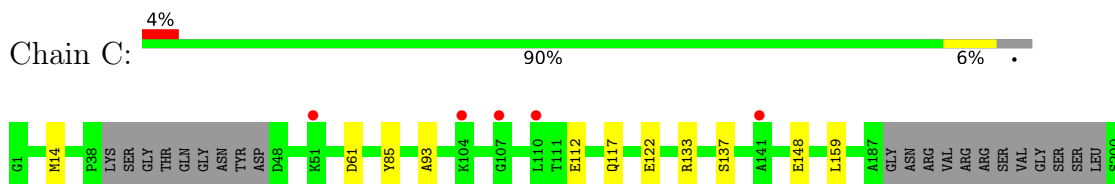
- Molecule 1: Diphtheria toxin

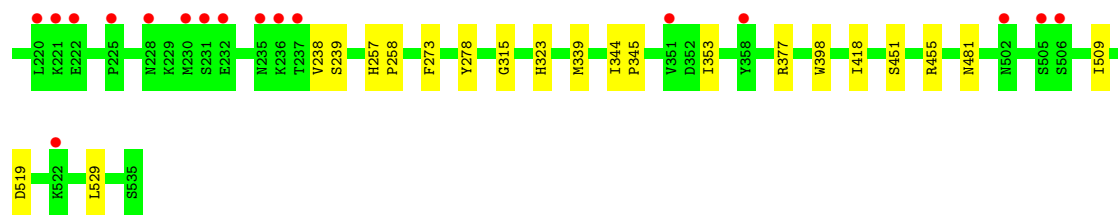


- Molecule 1: Diphtheria toxin

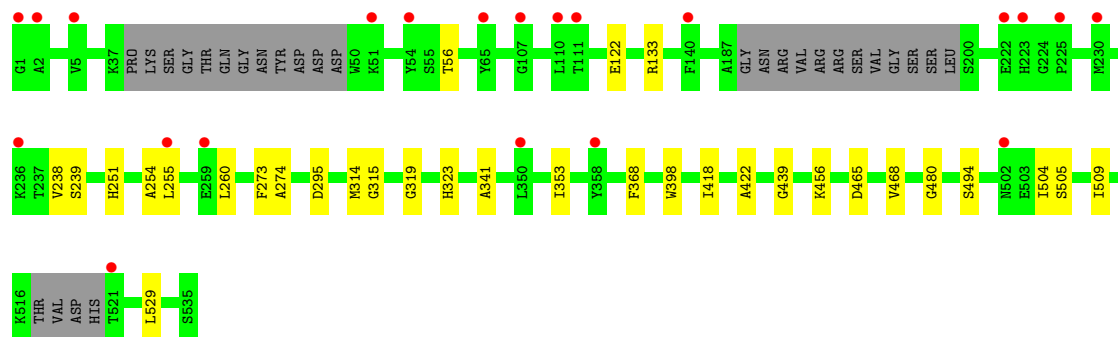
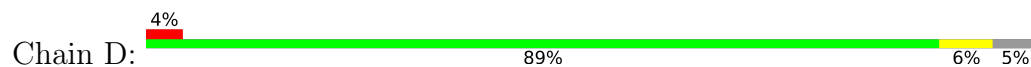


- Molecule 1: Diphtheria toxin





- Molecule 1: Diphtheria toxin



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.21Å 69.17Å 127.88Å 90.09° 90.01° 82.02°	Depositor
Resolution (Å)	29.08 – 2.35 29.08 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.08-2.35) 98.0 (29.08-2.35)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.36Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.207 , 0.250 0.207 , 0.248	Depositor DCC
$R_{free}$ test set	4932 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 24.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.437 for -h,-k,l 0.338 for k,h,-l 0.329 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.40	0/3991	0.57	0/5402
1	B	0.40	0/4013	0.56	0/5434
1	C	0.40	0/4038	0.57	0/5469
1	D	0.40	0/3997	0.57	0/5409
All	All	0.40	0/16039	0.57	0/21714

There are no bond length outliers.

There are no bond angle outliers.

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	3915	0	3859	22	0
1	B	3935	0	3873	36	0
1	C	3959	0	3895	20	0
1	D	3921	0	3861	19	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	B	6	0	8	0	0
4	A	94	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	88	0	0	2	0
4	C	91	0	0	1	0
4	D	80	0	0	1	0
All	All	16104	0	15496	93	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 3.

All (93) 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:65:TYR:OH	1:B:140:PHE:CZ	2.45	0.70
1:B:437:ILE:HD11	1:B:504:ILE:HG12	1.76	0.67
1:A:456:LYS:NZ	1:B:148:GLU:OE1	2.28	0.67
1:A:52:GLU:HG3	1:A:115:MET:HG3	1.79	0.65
1:D:122:GLU:OE1	1:D:122:GLU:N	2.27	0.61
1:D:273:PHE:CE1	1:D:315:GLY:HA2	2.37	0.60
1:B:315:GLY:HA3	1:B:323:HIS:CD2	2.37	0.59
1:C:315:GLY:HA3	1:C:323:HIS:CD2	2.39	0.58
1:D:295[A]:ASP:OD1	1:D:295[A]:ASP:O	2.21	0.58
1:D:315:GLY:HA3	1:D:323:HIS:CD2	2.39	0.57
1:B:273:PHE:CE1	1:B:315:GLY:HA2	2.39	0.57
1:C:238:VAL:HG22	1:C:239:SER:H	1.70	0.57
1:B:353:ILE:O	1:B:353:ILE:HG22	2.06	0.56
1:A:273:PHE:CE1	1:A:315:GLY:HA2	2.41	0.55
1:B:437:ILE:HD11	1:B:504:ILE:CG1	2.37	0.55
1:C:122:GLU:OE1	1:C:122:GLU:N	2.37	0.55
1:A:315:GLY:HA3	1:A:323:HIS:CD2	2.44	0.53
1:A:238:VAL:HG22	1:A:239:SER:N	2.24	0.52
1:D:418:ILE:HD13	1:D:529:LEU:HD13	1.91	0.52
1:A:418:ILE:HD13	1:A:529:LEU:CD1	2.40	0.52
1:D:422:ALA:HB3	1:D:480:GLY:HA2	1.91	0.51
1:B:238:VAL:HG22	1:B:239:SER:H	1.76	0.50
1:B:398:TRP:HH2	1:B:509:ILE:HD12	1.76	0.50
1:D:418:ILE:HD13	1:D:529:LEU:CD1	2.41	0.50
1:C:418:ILE:HD13	1:C:529:LEU:HD13	1.93	0.50
1:B:140:PHE:O	1:B:141:ALA:HB2	2.12	0.50
1:B:344:ILE:HB	1:B:345:PRO:HD3	1.94	0.50
1:D:465:ASP:OD1	1:D:468:VAL:N	2.44	0.49
1:A:61:ASP:OD1	1:A:377:ARG:NH1	2.44	0.48
1:B:54:TYR:HH	1:B:65:TYR:HD2	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LYS:HD3	1:A:497:GLU:HB2	1.95	0.48
1:C:451:SER:HA	1:C:455:ARG:O	2.14	0.48
1:B:226:ILE:HD11	1:B:257:HIS:HB2	1.95	0.48
1:A:199:LEU:O	1:A:200:SER:HB2	2.14	0.47
1:D:398:TRP:HH2	1:D:509:ILE:HD12	1.79	0.47
1:D:504:ILE:O	1:D:504:ILE:HG23	2.15	0.47
1:A:451:SER:O	1:A:485:ALA:HA	2.15	0.47
1:C:61:ASP:OD1	1:C:377:ARG:NH2	2.40	0.47
1:A:460:ARG:HD3	1:A:462:ARG:NH1	2.30	0.47
1:B:49:ASP:HA	1:B:113:PRO:HB3	1.95	0.47
1:A:418:ILE:HD13	1:A:529:LEU:HD12	1.96	0.47
1:B:255:LEU:HG	1:B:264:LYS:HD3	1.97	0.47
1:B:138:LEU:HD12	1:B:150:ILE:HD11	1.97	0.46
1:C:238:VAL:HG22	1:C:239:SER:N	2.31	0.46
1:B:85:TYR:CE2	1:B:159:LEU:HD21	2.50	0.46
1:A:255:LEU:HG	1:A:264:LYS:HD3	1.97	0.46
1:B:16:ASN:OD1	4:B:701:HOH:O	2.21	0.46
1:C:273:PHE:CE1	1:C:315:GLY:HA2	2.51	0.46
1:A:115:MET:O	1:A:152:ASN:ND2	2.49	0.45
1:B:238:VAL:HG22	1:B:239:SER:N	2.31	0.45
1:D:238:VAL:HG22	1:D:239:SER:N	2.30	0.45
1:B:451:SER:O	1:B:485:ALA:HA	2.15	0.45
1:C:278:TYR:HB3	1:C:339:MET:SD	2.56	0.44
1:B:251:HIS:CD2	1:B:335:LEU:HD21	2.53	0.44
1:D:439:GLY:O	1:D:494:SER:HB2	2.17	0.44
1:C:481:ASN:O	1:D:319:GLY:HA2	2.18	0.44
1:B:261:SER:O	1:B:264:LYS:HB3	2.16	0.44
1:B:65:TYR:OH	1:B:140:PHE:HZ	1.98	0.44
1:B:398:TRP:CH2	1:B:509:ILE:HD12	2.52	0.43
1:B:418:ILE:HG23	1:B:529:LEU:HD21	1.99	0.43
1:C:418:ILE:HD13	1:C:529:LEU:CD1	2.47	0.43
1:A:422:ALA:HB3	1:A:480:GLY:HA2	2.00	0.43
1:B:202:ILE:CD1	1:B:321:VAL:HG21	2.47	0.43
1:C:398:TRP:HH2	1:C:509:ILE:HD12	1.84	0.43
1:A:437:ILE:HD11	1:A:504:ILE:CG1	2.48	0.43
1:C:93:ALA:HA	1:C:137:SER:HB3	2.01	0.43
1:A:108:LEU:HB3	1:A:117:GLN:OE1	2.18	0.43
1:B:216:LYS:NZ	1:B:259:GLU:OE1	2.51	0.43
1:D:341:ALA:O	1:D:353:ILE:HD11	2.18	0.43
1:B:353:ILE:O	1:B:353:ILE:CG2	2.67	0.42
1:C:257:HIS:CD2	1:C:258:PRO:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ILE:HB	1:C:345:PRO:HD3	2.01	0.42
1:C:353:ILE:HG22	1:C:353:ILE:O	2.19	0.42
1:A:319:GLY:HA2	1:B:481:ASN:O	2.20	0.42
1:A:52:GLU:CG	1:A:115:MET:HG3	2.49	0.42
1:A:287:GLN:HG3	1:A:347:VAL:HG11	2.02	0.42
1:D:254:ALA:O	1:D:260:LEU:HD12	2.20	0.42
1:C:14:MET:HE1	4:C:770:HOH:O	2.19	0.42
1:D:274:ALA:HB1	4:D:772:HOH:O	2.20	0.41
1:B:470:PHE:CE2	1:B:472:ARG:CG	3.04	0.41
1:C:85:TYR:CE2	1:C:159:LEU:HD21	2.56	0.41
1:A:18:SER:HA	1:A:83:VAL:O	2.21	0.41
1:D:251:HIS:CE1	1:D:255:LEU:HD22	2.55	0.41
1:D:314:MET:HA	1:D:368:PHE:CE2	2.56	0.41
1:B:65:TYR:HH	1:B:140:PHE:HE1	1.60	0.41
1:B:407:ARG:O	1:B:493:ARG:NH2	2.54	0.40
1:B:470:PHE:CE2	1:B:472:ARG:HG2	2.57	0.40
1:B:202:ILE:HD11	1:B:321:VAL:HG21	2.03	0.40
1:C:112:GLU:O	1:C:117:GLN:NE2	2.42	0.40
1:B:29:ASP:HB2	4:B:722:HOH:O	2.22	0.40
1:B:94:LEU:HD13	1:B:102:ILE:HD13	2.02	0.40
1:A:22:GLY:HA3	1:A:62:ALA:O	2.21	0.40
1:C:148:GLU:OE2	1:D:456:LYS:NZ	2.53	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	501/535 (94%)	478 (95%)	23 (5%)	0	100 100
1	B	504/535 (94%)	481 (95%)	20 (4%)	3 (1%)	25 27
1	C	508/535 (95%)	485 (96%)	22 (4%)	1 (0%)	47 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	501/535 (94%)	479 (96%)	21 (4%)	1 (0%)	47 56
All	All	2014/2140 (94%)	1923 (96%)	86 (4%)	5 (0%)	47 56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	519	ASP
1	C	519	ASP
1	D	505	SER
1	B	141	ALA
1	B	503	GLU

### 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	431/453 (95%)	429 (100%)	2 (0%)	88 94
1	B	434/453 (96%)	432 (100%)	2 (0%)	88 94
1	C	436/453 (96%)	435 (100%)	1 (0%)	93 97
1	D	430/453 (95%)	428 (100%)	2 (0%)	88 94
All	All	1731/1812 (96%)	1724 (100%)	7 (0%)	91 95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	133	ARG
1	B	54	TYR
1	B	133	ARG
1	C	133	ARG
1	D	56	THR
1	D	133	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	HIS
1	A	520	HIS
1	B	323	HIS
1	C	384	HIS
1	D	251	HIS
1	D	323	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

4 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	C	601	-	4,4,4	0.34	0	6,6,6	0.16	0
2	SO4	B	601	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	D	601	-	4,4,4	0.33	0	6,6,6	0.15	0
3	GOL	B	602	-	5,5,5	0.37	0	5,5,5	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	602	-	-	0/4/4/4	-

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	509/535 (95%)	0.30	20 (3%) 39 52	35, 62, 108, 142	0
1	B	510/535 (95%)	0.24	23 (4%) 33 46	34, 59, 109, 135	0
1	C	514/535 (96%)	0.24	22 (4%) 35 47	36, 59, 112, 144	0
1	D	507/535 (94%)	0.23	21 (4%) 37 49	36, 62, 113, 148	0
All	All	2040/2140 (95%)	0.25	86 (4%) 36 48	34, 61, 112, 148	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	GLY	8.1
1	A	222	GLU	6.9
1	D	521	THR	5.9
1	C	222	GLU	5.8
1	D	502	ASN	5.7
1	A	51	LYS	5.6
1	C	221	LYS	5.6
1	B	226	ILE	5.5
1	D	2	ALA	4.9
1	C	351	VAL	4.9
1	B	51	LYS	4.8
1	C	231	SER	4.7
1	D	111	THR	4.6
1	B	351	VAL	4.5
1	D	51	LYS	4.4
1	A	104	LYS	4.3
1	D	358	TYR	4.3
1	C	228	ASN	4.2
1	B	222	GLU	4.2
1	B	286	ALA	4.1
1	B	246	TYR	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	502	ASN	4.0
1	A	358	TYR	4.0
1	B	228	ASN	4.0
1	B	350	LEU	4.0
1	B	104	LYS	3.9
1	A	199	LEU	3.7
1	C	505	SER	3.6
1	A	521	THR	3.6
1	B	225	PRO	3.5
1	D	236	LYS	3.4
1	C	502	ASN	3.3
1	B	54	TYR	3.3
1	C	51	LYS	3.3
1	C	141	ALA	3.2
1	D	222	GLU	3.2
1	C	236	LYS	3.2
1	B	223	HIS	3.2
1	C	235	ASN	3.2
1	C	506	SER	3.1
1	D	5	VAL	3.1
1	A	170	ARG	3.1
1	C	232	GLU	3.0
1	B	358	TYR	3.0
1	C	230	MET	3.0
1	C	220	LEU	2.9
1	A	346	LEU	2.9
1	B	123	PHE	2.9
1	B	520	HIS	2.9
1	C	522	LYS	2.8
1	D	230	MET	2.8
1	D	255	LEU	2.7
1	A	230	MET	2.6
1	C	107	GLY	2.6
1	B	229	LYS	2.6
1	A	9	SER	2.5
1	B	255	LEU	2.5
1	B	5	VAL	2.5
1	C	110	LEU	2.5
1	A	502	ASN	2.5
1	D	107	GLY	2.5
1	D	259	GLU	2.4
1	A	157	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	238	VAL	2.3
1	A	4	ASP	2.3
1	D	110	LEU	2.3
1	A	228	ASN	2.3
1	D	140	PHE	2.3
1	A	350	LEU	2.2
1	A	38	PRO	2.2
1	A	247	LEU	2.2
1	B	130	GLY	2.2
1	C	237	THR	2.2
1	D	54	TYR	2.2
1	A	353	ILE	2.2
1	B	504	ILE	2.2
1	C	104	LYS	2.2
1	D	350	LEU	2.2
1	B	241	GLU	2.1
1	B	237	THR	2.1
1	D	65	TYR	2.1
1	D	223	HIS	2.1
1	C	225	PRO	2.1
1	D	225	PRO	2.1
1	A	140	PHE	2.1
1	C	358	TYR	2.1

## 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<sup>th</sup> 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	602	6/6	0.82	0.16	70,80,82,83	0
2	SO4	D	601	5/5	0.85	0.13	109,110,114,117	0
2	SO4	B	601	5/5	0.86	0.20	86,90,96,99	0
2	SO4	C	601	5/5	0.95	0.11	88,92,95,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.