



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:23 PM GMT

PDB ID : 2WZQ  
Title : INSERTION MUTANT E173GP174 OF THE NS3 PROTEASE-HELICASE  
FROM DENGUE VIRUS  
Authors : Luo, D.; Wei, N.; Doan, D.; Paradkar, P.; Chong, Y.; Davidson, A.; Kotaka,  
M.; Lescar, J.; Vasudevan, S.  
Deposited on : 2009-12-02  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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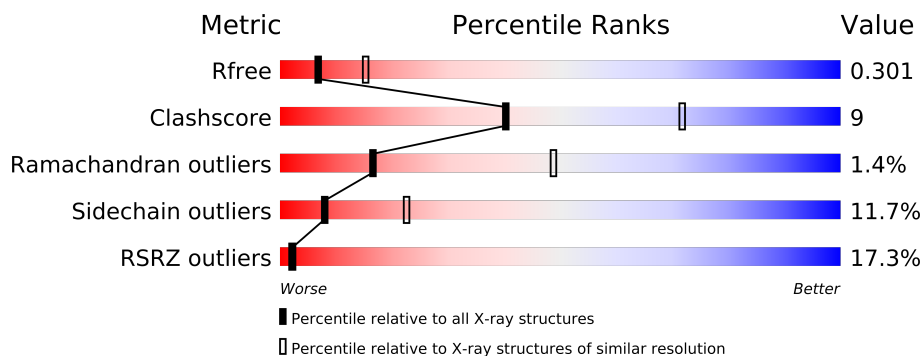
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	619	
2	C	31	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CL	A	1620	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4661 atoms, of which 0 are hydrogen and 0 are deuterium.

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 NS3 PROTEASE-HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4537	2861	809	846	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ASP	GLU	CONFLICT	UNP Q2TN89

- Molecule 2 is a protein called NS3 PROTEASE-HELICASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	0	0	0
			92	56	16	20			

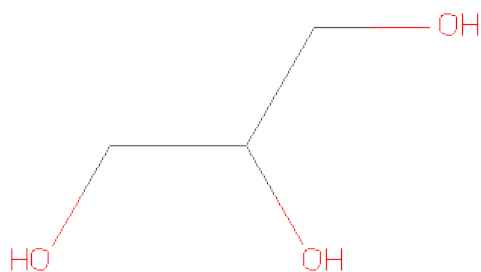
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	58	ASN	SER	CONFLICT	UNP Q2TN89
C	45	GLY	-	EXPRESSION TAG	UNP Q2TN89
C	46	SER	-	EXPRESSION TAG	UNP Q2TN89
C	47	ALA	-	EXPRESSION TAG	UNP Q2TN89
C	48	MET	-	EXPRESSION TAG	UNP Q2TN89
C	67	GLY	-	EXPRESSION TAG	UNP Q2TN89
C	68	GLY	-	EXPRESSION TAG	UNP Q2TN89
C	69	GLY	-	EXPRESSION TAG	UNP Q2TN89
C	70	GLY	-	EXPRESSION TAG	UNP Q2TN89
C	71	SER	-	EXPRESSION TAG	UNP Q2TN89
C	72	GLY	-	EXPRESSION TAG	UNP Q2TN89
C	73	GLY	-	EXPRESSION TAG	UNP Q2TN89
C	74	GLY	-	EXPRESSION TAG	UNP Q2TN89
C	75	GLY	-	EXPRESSION TAG	UNP Q2TN89

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 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
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

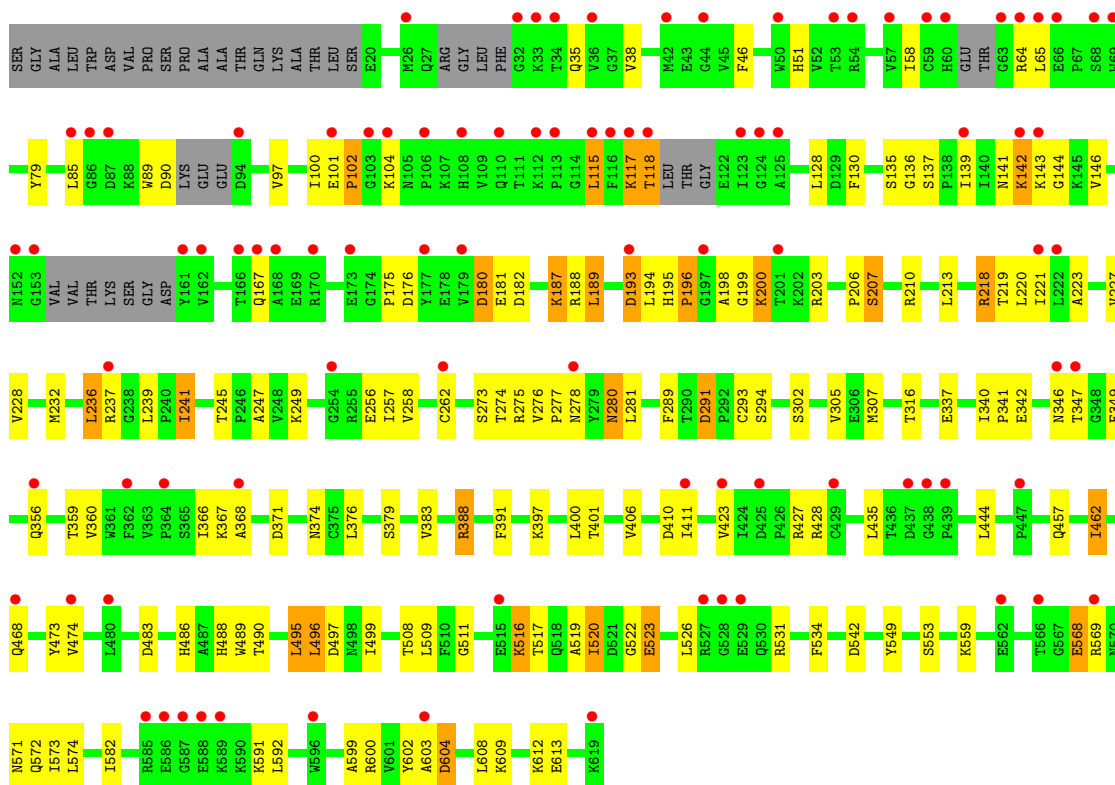
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

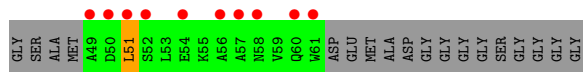
#### • Molecule 1: NS3 PROTEASE-HELICASE

Chain A: 



#### • Molecule 2: NS3 PROTEASE-HELICASE

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.42Å 87.72Å 75.78Å 90.00° 92.90° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.59 – 2.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.80) 98.6 (29.59-2.76)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.220 , 0.288 0.268 , 0.301	Depositor DCC
$R_{free}$ test set	881 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.0	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , -0.2	EDS
Estimated twinning fraction	0.041 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 17419 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	4661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL

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	0.47	0/4634	0.65	1/6272 (0.0%)
2	C	0.46	0/91	0.60	0/122
All	All	0.47	0/4725	0.65	1/6394 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	PRO	N-CA-CB	5.62	110.04	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4537	0	4468	86	2
2	C	92	0	89	1	0
3	A	1	0	0	0	0
4	A	6	0	8	1	0
5	A	25	0	0	2	0
All	All	4661	0	4565	86	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (86) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:GLU:HB3	1:A:182:ASP:CB	1.59	1.30
1:A:181:GLU:CB	1:A:182:ASP:HB3	1.69	1.23
1:A:423:VAL:HG23	1:A:462:ILE:HD13	1.54	0.90
1:A:520:ILE:O	1:A:523:GLU:HG2	1.84	0.78
1:A:599:ALA:HA	1:A:602:TYR:CE1	2.21	0.74
1:A:486:HIS:HD2	1:A:488:HIS:H	1.35	0.74
1:A:46:PHE:HB3	1:A:79:TYR:HB2	1.70	0.72
1:A:427:ARG:HD2	1:A:473:TYR:OH	1.94	0.67
1:A:573:ILE:HG13	1:A:592:LEU:HG	1.78	0.65
1:A:280:ASN:H	1:A:280:ASN:ND2	1.95	0.64
1:A:181:GLU:HB3	1:A:182:ASP:HB3	0.73	0.63
1:A:180:ASP:OD2	1:A:180:ASP:N	2.29	0.62
1:A:388:ARG:HG3	1:A:411:ILE:HD13	1.82	0.62
1:A:486:HIS:CD2	1:A:488:HIS:H	2.18	0.62
1:A:65:LEU:HD22	1:A:79:TYR:HB3	1.82	0.62
1:A:366:ILE:HD12	1:A:366:ILE:H	1.64	0.61
1:A:368:ALA:O	1:A:371:ASP:HB2	2.01	0.61
1:A:196:PRO:HA	1:A:200:LYS:HD3	1.82	0.60
1:A:280:ASN:H	1:A:280:ASN:HD22	1.48	0.59
1:A:51:HIS:HE1	1:A:135:SER:HB3	1.69	0.58
1:A:496:LEU:HA	1:A:499:ILE:HD12	1.85	0.57
1:A:38:VAL:O	1:A:136:GLY:HA3	2.03	0.57
1:A:526:LEU:O	1:A:531:ARG:HB2	2.04	0.57
1:A:245:THR:HG22	1:A:247:ALA:H	1.71	0.55
1:A:203:ARG:O	1:A:207:SER:HB2	2.06	0.55
1:A:360:VAL:HA	1:A:406:VAL:HG13	1.88	0.55
1:A:97:VAL:HG22	1:A:139:ILE:HG12	1.89	0.54
1:A:276:VAL:HG22	1:A:278:ASN:ND2	2.23	0.54
1:A:291:ASP:O	1:A:294:SER:HB2	2.09	0.53
1:A:218:ARG:NH1	1:A:280:ASN:OD1	2.42	0.53
1:A:206:PRO:HB2	1:A:210:ARG:HH12	1.74	0.53
1:A:388:ARG:NH2	1:A:410:ASP:OD1	2.42	0.52
1:A:236:LEU:HB3	1:A:241:ILE:HD13	1.91	0.52
1:A:293:CYS:HB2	5:A:2008:HOH:O	2.10	0.51
1:A:508:THR:HG22	1:A:509:LEU:N	2.26	0.51
1:A:89:TRP:CG	1:A:90:ASP:N	2.79	0.50
1:A:341:PRO:HD3	1:A:349:PHE:CE1	2.47	0.49
1:A:51:HIS:CE1	1:A:135:SER:HB3	2.47	0.49
1:A:218:ARG:N	1:A:280:ASN:HD21	2.09	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:346:ASN:O	1:A:347:THR:HG23	2.13	0.47
1:A:227:VAL:HG21	1:A:391:PHE:CE2	2.49	0.47
1:A:35:GLN:HB3	1:A:102:PRO:HB3	1.96	0.47
1:A:199:GLY:HA3	1:A:203:ARG:H	1.80	0.47
1:A:280:ASN:N	1:A:280:ASN:HD22	2.10	0.47
1:A:115:LEU:HD13	1:A:115:LEU:H	1.80	0.46
1:A:193:ASP:HA	1:A:316:THR:O	2.14	0.46
1:A:181:GLU:HB3	1:A:182:ASP:CA	2.36	0.46
1:A:141:ASN:O	1:A:143:LYS:N	2.47	0.46
1:A:397:LYS:O	1:A:401:THR:HG22	2.16	0.46
1:A:280:ASN:ND2	1:A:280:ASN:N	2.60	0.46
1:A:600:ARG:HD2	5:A:2022:HOH:O	2.16	0.46
1:A:228:VAL:HG12	1:A:232:MET:CE	2.47	0.45
1:A:603:ALA:O	1:A:604:ASP:HB3	2.17	0.45
1:A:187:LYS:HA	1:A:305:VAL:O	2.16	0.45
1:A:236:LEU:O	1:A:237:ARG:C	2.55	0.45
1:A:495:LEU:O	1:A:499:ILE:HD12	2.16	0.45
1:A:568:GLU:O	1:A:571:ASN:HB2	2.17	0.45
1:A:206:PRO:HB2	1:A:210:ARG:NH1	2.30	0.45
1:A:468:GLN:H	1:A:468:GLN:CD	2.21	0.45
1:A:223:ALA:O	1:A:262:CYS:HA	2.17	0.44
1:A:142:LYS:HD2	1:A:142:LYS:HA	1.86	0.44
1:A:572:GLN:OE1	1:A:591:LYS:HB3	2.17	0.44
1:A:51:HIS:CE1	1:A:135:SER:CB	3.01	0.44
1:A:117:LYS:O	1:A:118:THR:HG22	2.18	0.44
1:A:483:ASP:OD1	4:A:1621:GOL:O1	2.35	0.44
1:A:489:TRP:CE2	1:A:516:LYS:HG2	2.53	0.44
1:A:534:PHE:CD1	1:A:549:TYR:HA	2.53	0.44
1:A:198:ALA:HA	1:A:199:GLY:HA2	1.67	0.43
1:A:213:LEU:HD21	1:A:258:VAL:HG23	1.99	0.43
1:A:181:GLU:CB	1:A:182:ASP:CB	2.55	0.43
1:A:609:LYS:O	1:A:613:GLU:HG2	2.18	0.43
1:A:275:ARG:O	1:A:277:PRO:HD3	2.19	0.43
1:A:526:LEU:HD11	1:A:553:SER:HB3	2.01	0.43
1:A:101:GLU:HB2	1:A:104:LYS:HB2	2.00	0.43
1:A:519:ALA:HB1	1:A:523:GLU:OE1	2.19	0.42
1:A:128:LEU:HB3	1:A:130:PHE:CE1	2.54	0.42
1:A:340:ILE:HD11	1:A:474:VAL:HG12	2.00	0.42
1:A:219:THR:HG23	1:A:281:LEU:HD23	2.02	0.42
1:A:189:LEU:HD12	1:A:305:VAL:HG21	2.02	0.42
1:A:497:ASP:HB2	1:A:522:GLY:HA2	2.02	0.41
1:A:457:GLN:NE2	1:A:457:GLN:HA	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:38:VAL:HG21	1:A:100:ILE:HB	2.02	0.41
1:A:582:ILE:HD13	1:A:612:LYS:HB3	2.01	0.41
1:A:534:PHE:HD1	1:A:549:TYR:HA	1.86	0.41
1:A:359:THR:HG22	1:A:360:VAL:N	2.36	0.41
1:A:58:ILE:HG23	2:C:51:LEU:HD12	2.02	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273:SER:OG	1:A:337:GLU:OE1[1_655]	2.18	0.02
1:A:249:LYS:N	1:A:337:GLU:O[1_655]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	569/619 (92%)	509 (90%)	52 (9%)	8 (1%)	16	49
2	C	11/31 (36%)	10 (91%)	1 (9%)	0	100	100
All	All	580/650 (89%)	519 (90%)	53 (9%)	8 (1%)	16	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	PRO
1	A	200	LYS
1	A	142	LYS
1	A	176	ASP
1	A	144	GLY
1	A	194	LEU
1	A	218	ARG
1	A	511	GLY

### 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	A	478/524 (91%)	422 (88%)	56 (12%)	8	22
2	C	9/17 (53%)	8 (89%)	1 (11%)	9	25
All	All	487/541 (90%)	430 (88%)	57 (12%)	8	22

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	85	LEU
1	A	102	PRO
1	A	115	LEU
1	A	117	LYS
1	A	118	THR
1	A	137	SER
1	A	146	VAL
1	A	167	GLN
1	A	180	ASP
1	A	187	LYS
1	A	188	ARG
1	A	189	LEU
1	A	193	ASP
1	A	195	HIS
1	A	207	SER
1	A	220	LEU
1	A	221	ILE
1	A	236	LEU
1	A	239	LEU
1	A	241	ILE
1	A	256	GLU
1	A	257	ILE
1	A	274	THR
1	A	280	ASN
1	A	289	PHE
1	A	291	ASP
1	A	302	SER
1	A	307	MET

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Mol	Chain	Res	Type
1	A	342	GLU
1	A	356	GLN
1	A	367	LYS
1	A	374	ASN
1	A	376	LEU
1	A	379	SER
1	A	383	VAL
1	A	388	ARG
1	A	400	LEU
1	A	428	ARG
1	A	435	LEU
1	A	444	LEU
1	A	462	ILE
1	A	490	THR
1	A	495	LEU
1	A	496	LEU
1	A	516	LYS
1	A	517	THR
1	A	520	ILE
1	A	523	GLU
1	A	542	ASP
1	A	559	LYS
1	A	568	GLU
1	A	569	ARG
1	A	574	LEU
1	A	604	ASP
1	A	608	LEU
2	C	51	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	167	GLN
1	A	278	ASN
1	A	280	ASN
1	A	288	HIS
1	A	330	ASN
1	A	356	GLN
1	A	385	GLN
1	A	457	GLN
1	A	486	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
4	GOL	A	1621	-	5,5,5	0.32	0	5,5,5	0.40	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
4	GOL	A	1621	-	-	0/4/4/4	0/0/0/0

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	581/619 (93%)	1.21	93 (16%) 3 2	9, 23, 41, 62	1 (0%)
2	C	13/31 (41%)	3.44	10 (76%) 0 0	28, 29, 32, 32	0
All	All	594/650 (91%)	1.26	103 (17%) 2 2	9, 23, 41, 62	1 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	TYR	8.1
1	A	587	GLY	8.1
1	A	153	GLY	7.6
2	C	57	ALA	6.8
2	C	56	ALA	6.7
1	A	34	THR	6.5
1	A	103	GLY	5.9
1	A	162	VAL	5.9
1	A	168	ALA	5.9
1	A	59	CYS	5.6
1	A	63	GLY	5.4
1	A	33	LYS	5.1
2	C	50	ASP	4.8
1	A	201	THR	4.7
1	A	439	PRO	4.5
1	A	589	LYS	4.5
2	C	58	ASN	4.3
1	A	117	LYS	4.3
1	A	118	THR	4.2
1	A	32	GLY	4.1
1	A	125	ALA	4.0
1	A	529	GLU	4.0
1	A	26	MET	3.9
1	A	86	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	170	ARG	3.8
1	A	586	GLU	3.8
1	A	115	LEU	3.8
2	C	49	ALA	3.7
1	A	68	SER	3.7
1	A	112	LYS	3.7
1	A	437	ASP	3.6
1	A	69	TRP	3.6
1	A	87	ASP	3.6
1	A	468	GLN	3.5
2	C	61	TRP	3.5
1	A	101	GLU	3.4
1	A	106	PRO	3.4
1	A	108	HIS	3.3
1	A	166	THR	3.3
1	A	54	ARG	3.3
1	A	94	ASP	3.3
2	C	60	GLN	3.3
1	A	116	PHE	3.2
1	A	60	HIS	3.2
1	A	346	ASN	3.1
1	A	569	ARG	3.1
1	A	585	ARG	3.0
1	A	104	LYS	3.0
1	A	65	LEU	3.0
1	A	179	VAL	3.0
2	C	51	LEU	3.0
1	A	193	ASP	2.9
1	A	113	PRO	2.8
1	A	356	GLN	2.8
1	A	411	ILE	2.8
1	A	85	LEU	2.8
1	A	167	GLN	2.7
1	A	42	MET	2.7
1	A	123	ILE	2.6
2	C	54	GLU	2.6
1	A	528	GLY	2.6
1	A	66	GLU	2.6
1	A	152	ASN	2.6
1	A	44	GLY	2.6
1	A	480	LEU	2.5
1	A	596	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	222	LEU	2.5
1	A	53	THR	2.5
1	A	50	TRP	2.5
1	A	110	GLN	2.4
1	A	221	ILE	2.4
1	A	64	ARG	2.4
1	A	177	TYR	2.4
1	A	173	GLU	2.4
1	A	139	ILE	2.4
1	A	527	ARG	2.4
1	A	515	GLU	2.4
1	A	368	ALA	2.3
1	A	474	VAL	2.3
1	A	36	VAL	2.3
1	A	429	CYS	2.3
1	A	588	GLU	2.3
1	A	347	THR	2.2
1	A	438	GLY	2.2
1	A	262	CYS	2.2
1	A	562	GLU	2.2
1	A	362	PHE	2.2
1	A	142	LYS	2.2
1	A	278	ASN	2.1
1	A	143	LYS	2.1
1	A	364	PRO	2.1
1	A	254	GLY	2.1
1	A	603	ALA	2.1
1	A	124	GLY	2.1
1	A	197	GLY	2.1
2	C	52	SER	2.1
1	A	423	VAL	2.0
1	A	425	ASP	2.0
1	A	566	THR	2.0
1	A	57	VAL	2.0
1	A	447	PRO	2.0
1	A	237	ARG	2.0
1	A	619	LYS	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

There are no carbohydrates in this entry.

### 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	A	1620	1/1	0.36	3.71	74,74,74,74	0
4	GOL	A	1621	6/6	0.27	1.09	41,41,42,43	0

### 6.5 Other polymers

There are no such residues in this entry.