



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2024 – 07:54 PM EDT

PDB ID : 2B20  
Title : Crystal Structure of Enterochelin Esterase from *Shigella flexneri* Enterochelin Esterase  
Authors : Kim, Y.; Maltseva, N.; Dementieva, I.; Quartey, P.; Holzle, D.; Collart, F.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2005-09-16  
Resolution : 2.95 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>.

---

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

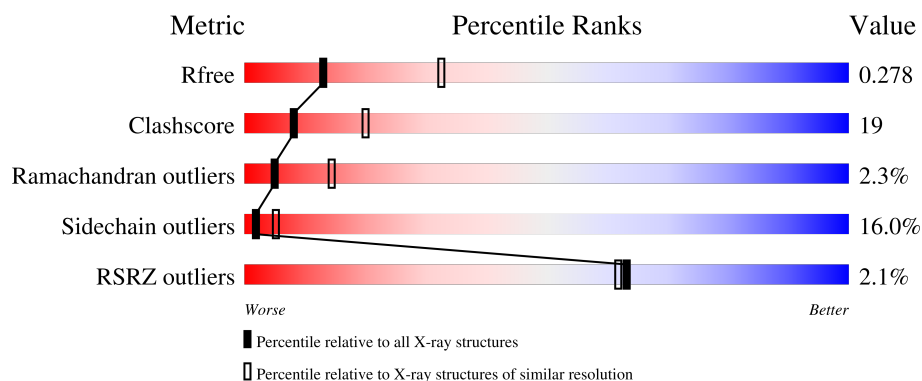
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

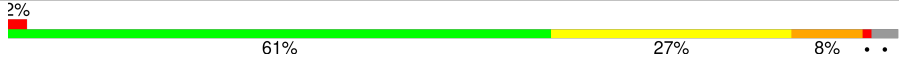
The reported resolution of this entry is 2.95 Å.

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))
$R_{free}$	164625	1044 (2.98-2.94)
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)
RSRZ outliers	164620	1044 (2.98-2.94)

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	403	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3278 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.

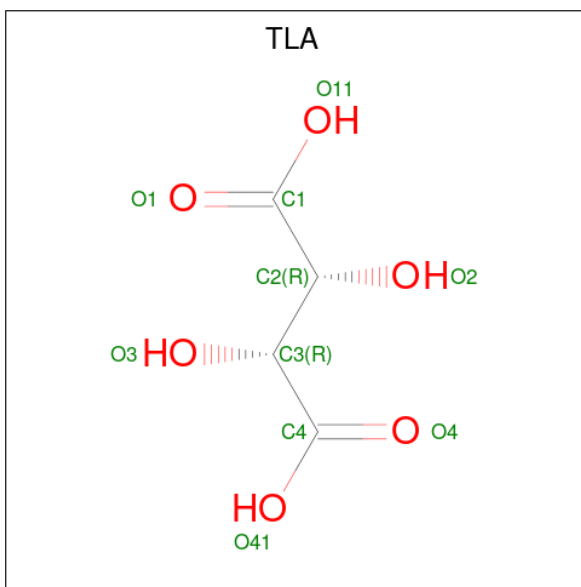
- Molecule 1 is a protein called enterochelin esterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	Se	0	6	0
			3218	2066	571	569	5	7			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	cloning artifact	UNP Q83SB9
A	-1	ASN	-	cloning artifact	UNP Q83SB9
A	0	ALA	-	cloning artifact	UNP Q83SB9
A	1	MSE	MET	modified residue	UNP Q83SB9
A	27	MSE	MET	modified residue	UNP Q83SB9
A	68	MSE	MET	modified residue	UNP Q83SB9
A	146	MSE	MET	modified residue	UNP Q83SB9
A	209	MSE	MET	modified residue	UNP Q83SB9
A	347	MSE	MET	modified residue	UNP Q83SB9
A	349	MSE	MET	modified residue	UNP Q83SB9
A	385	MSE	MET	modified residue	UNP Q83SB9

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		

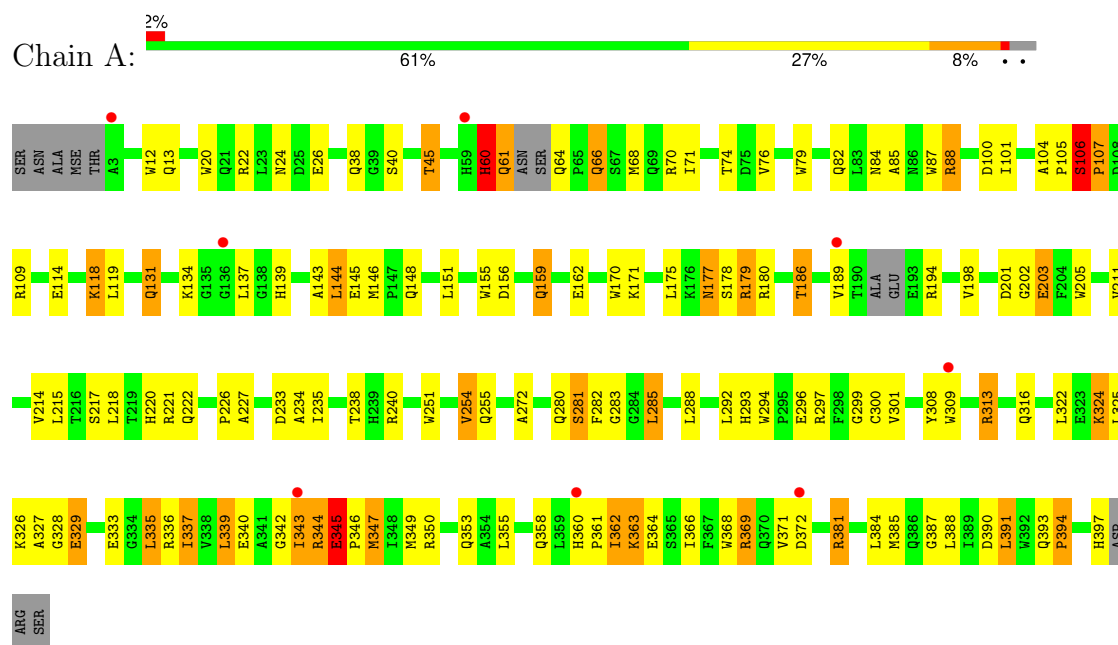
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		

### 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: enterochelin esterase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.17Å 66.17Å 252.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.11 – 2.95 40.11 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.11-2.95) 99.6 (40.11-2.95)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005, CNS	Depositor
R, $R_{free}$	0.222 , 0.277 0.219 , 0.278	Depositor DCC
$R_{free}$ test set	611 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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

### 5.1 Standard geometry

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

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	0.61	0/3318	0.72	1/4518 (0.0%)

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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	335	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	345	GLU	Peptide

### 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	3218	0	3096	120	0
2	A	10	0	4	1	0
3	A	50	0	0	7	0
All	All	3278	0	3100	121	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 19.

All (121) 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:A:186:THR:HG22	1:A:227:ALA:H	1.06	1.18
1:A:106:SER:HB2	1:A:107:PRO:HA	1.22	1.09
1:A:38:GLN:NE2	1:A:45:THR:HG22	1.72	1.02
1:A:38:GLN:HE22	1:A:45:THR:HG22	0.89	1.02
1:A:66[A]:GLN:H	1:A:66[A]:GLN:NE2	1.63	0.96
1:A:235:ILE:N	3:A:517:HOH:O	1.95	0.94
1:A:106:SER:HB2	1:A:107:PRO:CA	1.99	0.92
1:A:38:GLN:HE22	1:A:45:THR:CG2	1.81	0.92
1:A:369:ARG:NH2	1:A:390:ASP:OD1	2.02	0.92
1:A:114:GLU:HG3	1:A:118:LYS:HE2	1.52	0.91
1:A:215:LEU:HD23	1:A:385:MSE:HE1	1.53	0.91
1:A:66[A]:GLN:HE21	1:A:66[A]:GLN:N	1.69	0.90
1:A:22:ARG:HD2	1:A:24:ASN:O	1.72	0.89
1:A:186:THR:HG22	1:A:227:ALA:N	1.89	0.87
1:A:218:LEU:HD12	1:A:385:MSE:HE2	1.58	0.85
1:A:218:LEU:HD12	1:A:385:MSE:CE	2.08	0.83
1:A:313:ARG:HG3	1:A:313:ARG:HH11	1.43	0.83
1:A:186:THR:HG21	3:A:530:HOH:O	1.78	0.82
1:A:309[B]:TRP:CD1	1:A:347:MSE:SE	2.85	0.80
1:A:313:ARG:HH11	1:A:313:ARG:CG	1.95	0.79
1:A:203:GLU:HG3	1:A:233:ASP:OD2	1.82	0.78
1:A:361:PRO:HB2	1:A:362:ILE:HD13	1.66	0.78
1:A:393:GLN:HB3	1:A:394:PRO:HD3	1.65	0.78
1:A:272:ALA:HB2	1:A:296:GLU:O	1.83	0.77
1:A:360[A]:HIS:CG	1:A:361:PRO:HD3	2.22	0.75
1:A:186:THR:CG2	1:A:227:ALA:H	1.94	0.75
1:A:66[A]:GLN:H	1:A:66[A]:GLN:HE21	0.83	0.73
1:A:347:MSE:HE2	1:A:350:ARG:NH1	2.07	0.70
1:A:309[B]:TRP:HD1	1:A:347:MSE:SE	2.22	0.70
1:A:60:HIS:O	1:A:61:GLN:HB2	1.91	0.69
1:A:322:LEU:HD21	1:A:355:LEU:HA	1.76	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ALA:O	1:A:299:GLY:HA3	1.93	0.67
1:A:346:PRO:HD2	1:A:347:MSE:H	1.60	0.66
1:A:186:THR:HG23	1:A:226:PRO:HA	1.77	0.66
1:A:393:GLN:HB3	1:A:394:PRO:CD	2.26	0.66
1:A:24:ASN:HD22	1:A:26:GLU:H	1.43	0.66
1:A:300:CYS:HB3	1:A:391:LEU:HG	1.77	0.65
1:A:88:ARG:HB2	1:A:145:GLU:HG2	1.79	0.65
1:A:203:GLU:CG	1:A:233:ASP:OD2	2.44	0.64
1:A:344:ARG:HD2	1:A:372:ASP:O	1.98	0.62
1:A:339:LEU:HD11	1:A:355:LEU:HD23	1.82	0.62
2:A:501:TLA:H2	3:A:531:HOH:O	1.99	0.61
1:A:186:THR:CG2	1:A:226:PRO:HA	2.30	0.61
1:A:313:ARG:HH11	1:A:313:ARG:CB	2.14	0.61
1:A:177:ASN:C	1:A:177:ASN:HD22	2.05	0.60
1:A:87:TRP:HZ3	1:A:144:LEU:HB3	1.66	0.59
1:A:171:LYS:HG3	1:A:178:SER:OG	2.02	0.59
1:A:346:PRO:CD	1:A:347:MSE:H	2.11	0.59
1:A:12:TRP:CZ2	1:A:76:VAL:HG22	2.38	0.59
1:A:68:MSE:HG2	1:A:79:TRP:HB2	1.85	0.58
1:A:170:TRP:CE3	1:A:179:ARG:HD3	2.38	0.58
1:A:362:ILE:O	1:A:364:GLU:N	2.37	0.58
1:A:326:LYS:C	1:A:328:GLY:H	2.08	0.57
1:A:179:ARG:HD2	3:A:516:HOH:O	2.05	0.57
1:A:205:TRP:HE1	1:A:280:GLN:HE22	1.52	0.56
1:A:101:ILE:HG21	1:A:119:LEU:HD21	1.88	0.56
1:A:301:VAL:HB	1:A:337:ILE:HB	1.88	0.56
1:A:24:ASN:ND2	1:A:26:GLU:H	2.04	0.56
1:A:281:SER:OG	1:A:282:PHE:N	2.39	0.55
1:A:218:LEU:HD12	1:A:385:MSE:HE3	1.86	0.54
1:A:64:GLN:HB2	1:A:106:SER:O	2.09	0.53
1:A:155:TRP:CE3	1:A:214:VAL:HG21	2.43	0.53
1:A:88:ARG:NH2	1:A:145:GLU:OE1	2.40	0.53
1:A:360[A]:HIS:CD2	1:A:361:PRO:HD3	2.43	0.53
1:A:66[A]:GLN:HB2	1:A:79:TRP:HE1	1.74	0.53
1:A:393:GLN:HA	1:A:393:GLN:OE1	2.09	0.52
1:A:106:SER:CB	1:A:107:PRO:HA	2.14	0.52
1:A:360[B]:HIS:HA	1:A:363:LYS:HG3	1.90	0.52
1:A:177:ASN:ND2	3:A:516:HOH:O	2.42	0.52
1:A:162:GLU:OE1	1:A:220[B]:HIS:HE1	1.94	0.51
1:A:360[A]:HIS:CD2	1:A:360[A]:HIS:H	2.28	0.51
1:A:155:TRP:CZ2	1:A:381:ARG:HB2	2.47	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:HH11	1:A:344:ARG:HB3	1.77	0.50
1:A:342:GLY:O	1:A:345:GLU:HG2	2.12	0.49
1:A:159:GLN:HG3	1:A:217:SER:HA	1.94	0.49
1:A:131:GLN:HG2	1:A:143:ALA:HB2	1.94	0.48
1:A:234:ALA:CA	3:A:517:HOH:O	2.61	0.48
1:A:346:PRO:CD	1:A:347:MSE:N	2.77	0.47
1:A:101:ILE:HG13	1:A:101:ILE:O	2.15	0.47
1:A:40:SER:HA	1:A:74:THR:O	2.15	0.47
1:A:137:LEU:HB2	1:A:139:HIS:CD2	2.49	0.47
1:A:205:TRP:HE1	1:A:280:GLN:NE2	2.13	0.47
1:A:155:TRP:CE2	1:A:381:ARG:HB2	2.50	0.47
1:A:360[B]:HIS:N	1:A:361:PRO:CD	2.77	0.47
1:A:162:GLU:OE1	1:A:220[B]:HIS:CE1	2.68	0.46
1:A:360[A]:HIS:N	1:A:361:PRO:CD	2.77	0.46
1:A:251:TRP:HA	1:A:254:VAL:HG13	1.96	0.46
1:A:255:GLN:HE21	1:A:297:ARG:HG2	1.81	0.46
1:A:313:ARG:HG3	1:A:313:ARG:NH1	2.16	0.45
1:A:285:LEU:HD23	1:A:308:TYR:CD1	2.51	0.45
1:A:324:LYS:O	1:A:329:GLU:HB3	2.15	0.45
1:A:349:MSE:HE1	1:A:368:TRP:CZ2	2.52	0.45
1:A:309[B]:TRP:HA	1:A:309[B]:TRP:CE3	2.52	0.45
1:A:85:ALA:HB1	1:A:148:GLN:HG3	1.99	0.45
1:A:325:LEU:O	1:A:328:GLY:N	2.50	0.45
1:A:309[B]:TRP:HA	1:A:309[B]:TRP:HE3	1.82	0.44
1:A:343:ILE:H	1:A:343:ILE:HG13	1.55	0.44
1:A:361:PRO:HB2	1:A:362:ILE:CD1	2.42	0.44
1:A:337:ILE:HG12	1:A:366:ILE:HG12	1.99	0.44
1:A:221:ARG:C	1:A:222:GLN:HG2	2.37	0.43
1:A:393:GLN:CB	1:A:394:PRO:CD	2.92	0.43
1:A:240:ARG:HB3	3:A:537:HOH:O	2.17	0.43
1:A:201:ASP:OD1	1:A:240:ARG:HD2	2.17	0.43
1:A:20:TRP:CE3	1:A:146:MSE:HE1	2.54	0.43
1:A:179:ARG:HB2	1:A:233:ASP:HB3	1.99	0.43
1:A:12:TRP:HZ2	1:A:76:VAL:HG22	1.81	0.43
1:A:313:ARG:CB	1:A:313:ARG:NH1	2.80	0.43
1:A:233:ASP:OD2	1:A:234:ALA:O	2.36	0.42
1:A:293:HIS:HB2	1:A:294:TRP:CE3	2.55	0.42
1:A:104:ALA:HA	1:A:105:PRO:HD3	1.91	0.42
1:A:177:ASN:HD21	1:A:179:ARG:HH11	1.67	0.42
1:A:344:ARG:HB3	1:A:344:ARG:NH1	2.35	0.42
1:A:70:ARG:HG2	1:A:71:ILE:N	2.35	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLY:O	1:A:391:LEU:HD22	2.20	0.42
1:A:280:GLN:O	1:A:283:GLY:N	2.52	0.41
1:A:180:ARG:O	1:A:233:ASP:HB2	2.20	0.41
1:A:146:MSE:HA	1:A:146:MSE:HE2	2.02	0.40
1:A:202:GLY:O	1:A:203:GLU:C	2.57	0.40
1:A:349:MSE:HE3	1:A:349:MSE:O	2.21	0.40
1:A:349:MSE:HE2	1:A:353:GLN:OE1	2.22	0.40
1:A:101:ILE:HD11	1:A:118:LYS:HE3	2.04	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	391/403 (97%)	350 (90%)	32 (8%)	9 (2%)	<b>5</b> <b>14</b>

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	189	VAL
1	A	363	LYS
1	A	60	HIS
1	A	316	GLN
1	A	327	ALA
1	A	107	PRO
1	A	345	GLU
1	A	394	PRO

### 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	337/333 (101%)	282 (84%)	55 (16%)	<b>2</b> <b>5</b>

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	45	THR
1	A	60	HIS
1	A	61	GLN
1	A	66[A]	GLN
1	A	66[B]	GLN
1	A	82	GLN
1	A	84	ASN
1	A	88	ARG
1	A	100	ASP
1	A	106	SER
1	A	109	ARG
1	A	118	LYS
1	A	131	GLN
1	A	134	LYS
1	A	144	LEU
1	A	151	LEU
1	A	156[A]	ASP
1	A	156[B]	ASP
1	A	159	GLN
1	A	175	LEU
1	A	177	ASN
1	A	179	ARG
1	A	186	THR
1	A	194	ARG
1	A	198	VAL
1	A	203	GLU
1	A	211	VAL
1	A	238	THR
1	A	254	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	281	SER
1	A	285	LEU
1	A	288	LEU
1	A	292	LEU
1	A	313	ARG
1	A	324	LYS
1	A	329	GLU
1	A	333	GLU
1	A	335	LEU
1	A	336	ARG
1	A	337	ILE
1	A	339	LEU
1	A	340	GLU
1	A	343	ILE
1	A	344	ARG
1	A	347	MSE
1	A	358	GLN
1	A	362	ILE
1	A	369	ARG
1	A	371	VAL
1	A	381	ARG
1	A	384	LEU
1	A	388	LEU
1	A	391	LEU
1	A	397	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	38	GLN
1	A	61	GLN
1	A	82	GLN
1	A	131	GLN
1	A	139	HIS
1	A	159	GLN
1	A	177	ASN
1	A	255	GLN
1	A	280	GLN
1	A	304	GLN
1	A	386	GLN

### 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 ⓘ

1 ligand is 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	TLA	A	501	-	9,9,9	1.31	0	12,12,12	1.68	4 (33%)

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
2	TLA	A	501	-	-	4/12/12/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	TLA	O3-C3-C2	2.64	115.55	110.17
2	A	501	TLA	C3-C2-C1	2.46	115.27	109.82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	TLA	O2-C2-C3	2.42	115.09	110.17
2	A	501	TLA	O41-C4-C3	2.23	119.51	113.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	TLA	C2-C3-C4-O4
2	A	501	TLA	C2-C3-C4-O41
2	A	501	TLA	O11-C1-C2-C3
2	A	501	TLA	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	TLA	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, 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	384/403 (95%)	-0.10	8 (2%) 63 62	39, 76, 116, 132	6 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309[A]	TRP	7.7
1	A	59[A]	HIS	3.6
1	A	136	GLY	3.3
1	A	360[A]	HIS	3.1
1	A	189	VAL	2.8
1	A	3	ALA	2.5
1	A	372	ASP	2.4
1	A	343	ILE	2.2

### 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.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TLA	A	501	10/10	0.82	0.09	89,90,91,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.