



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 10:48 AM BST

PDB ID : 6UNW  
Title : Epoxide hydrolase from an endophytic Streptomyces  
Authors : Wilson, C.; dos Santos, J.C.; Dias, M.V.B.  
Deposited on : 2019-10-13  
Resolution : 2.21 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 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 : 2.14.4.dev1  
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) : 2.14.4.dev1

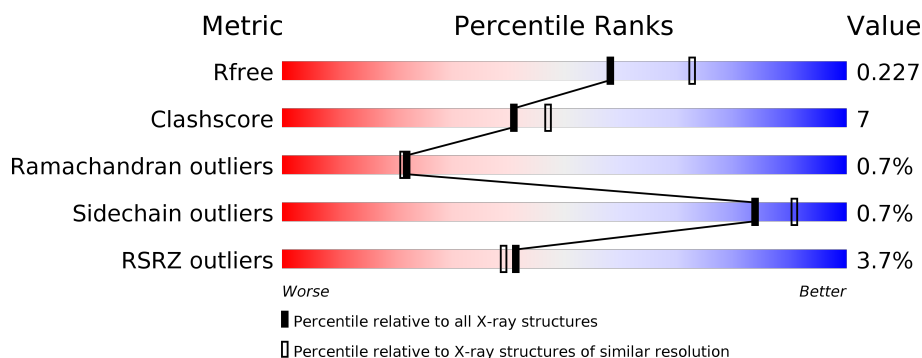
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 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	353	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>•• 6%</div> </div> </div>
1	B	353	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>• 9%</div> </div> </div>
1	C	353	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•• 9%</div> </div> </div>

## 2 Entry composition [i](#)

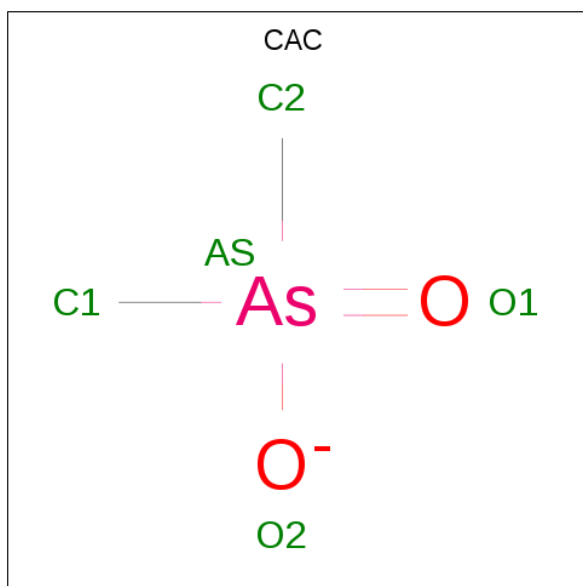
There are 4 unique types of molecules in this entry. The entry contains 8098 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Soluble epoxide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2553	1620	463	467	3			
1	B	322	Total	C	N	O	S	0	0	0
			2471	1571	441	456	3			
1	C	320	Total	C	N	O	S	0	1	0
			2461	1565	441	452	3			

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula:  $\text{C}_2\text{H}_6\text{AsO}_2$ ).



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

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

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

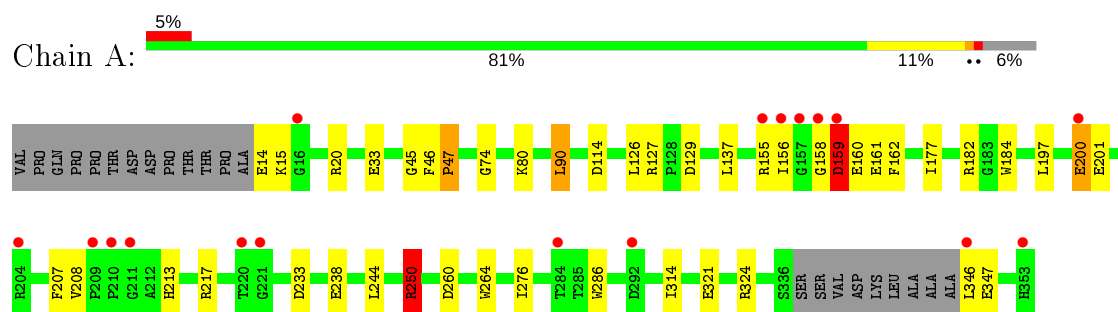
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	210	Total 210	O 210	0	0
4	B	209	Total 209	O 209	0	0
4	C	174	Total 174	O 174	0	0

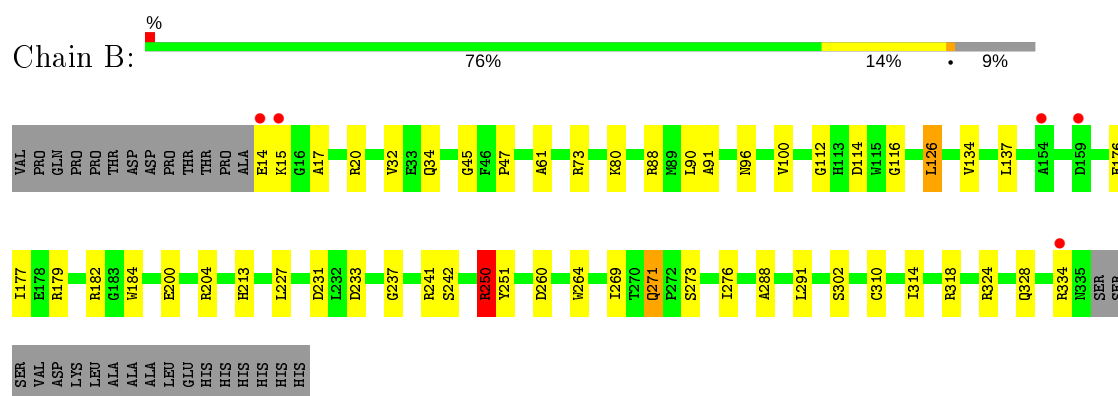
### 3 Residue-property plots

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.

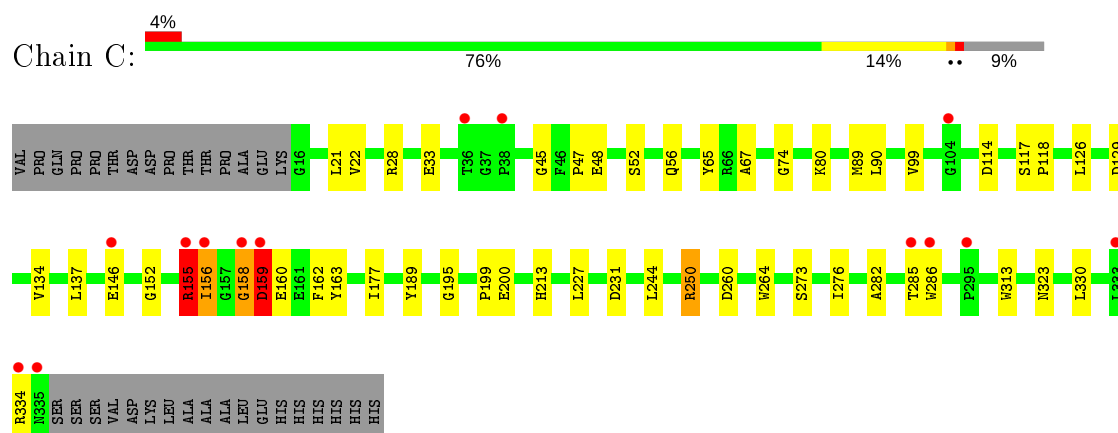
- Molecule 1: Soluble epoxide hydrolase



- Molecule 1: Soluble epoxide hydrolase



- Molecule 1: Soluble epoxide hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.73 Å   106.73 Å   233.04 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.52 – 2.21 48.52 – 2.21	Depositor EDS
% Data completeness (in resolution range)	94.9 (48.52-2.21) 95.4 (48.52-2.21)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.22 Å)	Xtriage
Refinement program	PHENIX 18.1-3865	Depositor
R, $R_{free}$	0.187 , 0.227 0.187 , 0.227	Depositor DCC
$R_{free}$ test set	3286 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8098	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: CAC, 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	0.51	0/2634	0.69	3/3602 (0.1%)
1	B	0.45	0/2547	0.71	5/3485 (0.1%)
1	C	0.50	1/2540 (0.0%)	0.86	6/3476 (0.2%)
All	All	0.49	1/7721 (0.0%)	0.75	14/10563 (0.1%)

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	2
1	B	0	1
1	C	0	4
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	146	GLU	CD-OE1	6.90	1.33	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	ASP	CB-CG-OD2	-22.96	97.64	118.30
1	C	159	ASP	CB-CG-OD1	12.73	129.76	118.30
1	B	20	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	B	250	ARG	NE-CZ-NH1	-7.82	116.39	120.30
1	B	20	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	C	158	GLY	C-N-CA	-6.66	105.06	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	250	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	C	155	ARG	CB-CG-CD	5.54	126.01	111.60
1	A	250	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	200	GLU	CA-CB-CG	-5.37	101.58	113.40
1	C	156	ILE	CG1-CB-CG2	-5.32	99.69	111.40
1	A	90	LEU	CA-CB-CG	-5.28	103.16	115.30
1	B	271	GLN	CB-CA-C	-5.09	100.21	110.40
1	B	126	LEU	CB-CG-CD2	5.06	119.59	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	GLY	Peptide
1	A	250	ARG	Sidechain
1	B	250	ARG	Sidechain
1	C	155	ARG	Sidechain
1	C	158	GLY	Peptide
1	C	159	ASP	Sidechain
1	C	199	PRO	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	2553	0	2415	35	0
1	B	2471	0	2352	36	0
1	C	2461	0	2346	36	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	210	0	0	2	0
4	B	209	0	0	1	1
4	C	174	0	0	3	1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8098	0	7113	104	1

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 7.

All (104) 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:159:ASP:OD1	1:A:160:GLU:N	1.92	1.02
1:A:321:GLU:OE2	1:A:324:ARG:NH2	2.06	0.88
1:A:197:LEU:HB3	1:A:201:GLU:HG3	1.59	0.83
1:C:159:ASP:OD1	1:C:160:GLU:N	2.12	0.83
1:A:346:LEU:HD23	1:A:347:GLU:H	1.42	0.82
1:B:251:TYR:OH	2:B:401:CAC:O2	2.01	0.79
1:B:250:ARG:HA	1:B:250:ARG:HE	1.56	0.70
1:A:14:GLU:HG3	1:A:15:LYS:HG3	1.74	0.70
1:A:276:ILE:HG22	1:A:314:ILE:HD11	1.75	0.68
1:B:126:LEU:HD22	1:B:264:TRP:CE2	2.30	0.67
1:A:14:GLU:N	4:A:501:HOH:O	2.29	0.65
1:A:74:GLY:HA2	1:A:80:LYS:HG2	1.80	0.64
1:C:156:ILE:HD11	1:C:162:PHE:CG	2.32	0.64
1:C:137:LEU:HD22	1:C:276:ILE:HB	1.80	0.64
1:C:126:LEU:HD22	1:C:264:TRP:CE2	2.32	0.64
1:A:160:GLU:OE1	1:A:217:ARG:NH1	2.27	0.64
1:A:238:GLU:OE2	1:B:241:ARG:NH1	2.30	0.63
1:C:250:ARG:HA	1:C:250:ARG:HE	1.64	0.62
1:A:250:ARG:HA	1:A:250:ARG:HE	1.65	0.61
1:C:250:ARG:CA	1:C:250:ARG:HE	2.14	0.61
1:B:45:GLY:HA3	1:B:114:ASP:HB3	1.83	0.59
1:B:14:GLU:HG2	1:B:15:LYS:HD2	1.85	0.58
1:A:159:ASP:OD1	1:A:160:GLU:HG3	2.05	0.57
1:A:160:GLU:HB3	1:A:207:PHE:HB3	1.88	0.56
1:C:163:TYR:OH	2:C:401:CAC:O2	2.21	0.56
1:A:213:HIS:HE1	4:A:652:HOH:O	1.89	0.56
1:A:45:GLY:HA3	1:A:114:ASP:HB3	1.89	0.55
1:C:195:GLY:HA2	4:C:599:HOH:O	2.06	0.55
1:B:126:LEU:HD22	1:B:264:TRP:CZ2	2.41	0.55
1:A:126:LEU:HD22	1:A:264:TRP:CE2	2.43	0.54
1:B:177:ILE:HG12	1:B:184:TRP:CE2	2.43	0.53
1:C:285:THR:HG23	1:C:286:TRP:HD1	1.74	0.53
1:A:161:GLU:HB3	1:A:208:VAL:HG13	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLN:HG2	1:B:61:ALA:HB2	1.91	0.53
1:A:20:ARG:NH1	1:A:33:GLU:OE1	2.43	0.52
1:C:213:HIS:HD2	4:C:502:HOH:O	1.92	0.52
1:A:127:ARG:NH2	1:A:129:ASP:OD2	2.42	0.52
1:C:89:MET:HE2	1:C:250:ARG:HH12	1.75	0.51
1:B:276:ILE:HG22	1:B:314:ILE:HD11	1.93	0.51
1:A:155:ARG:HG3	1:A:155:ARG:HH11	1.75	0.50
1:A:156:ILE:HG22	1:A:207:PHE:HE1	1.76	0.50
1:B:80:LYS:HE2	1:B:242:SER:HB2	1.93	0.50
1:B:182:ARG:NH1	1:B:233:ASP:OD2	2.41	0.50
1:C:74:GLY:HA2	1:C:80:LYS:HG2	1.94	0.49
1:C:33:GLU:HA	1:C:67:ALA:O	2.13	0.49
1:B:324:ARG:NH1	1:B:328:GLN:OE1	2.46	0.48
1:C:22:VAL:HG21	1:C:99:VAL:HG22	1.95	0.48
1:C:45:GLY:HA3	1:C:114:ASP:HB3	1.95	0.48
1:B:176:GLU:O	1:B:179:ARG:HD3	2.12	0.48
1:A:156:ILE:HG22	1:A:207:PHE:CE1	2.49	0.48
1:B:288:ALA:HA	1:B:291:LEU:HD12	1.96	0.48
1:C:89:MET:CE	1:C:250:ARG:HH12	2.27	0.48
1:B:237:GLY:O	1:B:241:ARG:HG3	2.13	0.47
1:A:177:ILE:HG21	1:A:244:LEU:HG	1.96	0.47
1:B:200:GLU:HB3	1:B:204:ARG:NH1	2.30	0.47
1:A:90:LEU:HD13	1:A:260:ASP:HB3	1.96	0.47
1:B:250:ARG:CA	1:B:250:ARG:HE	2.26	0.47
1:C:126:LEU:HD22	1:C:264:TRP:CZ2	2.49	0.47
1:A:162:PHE:CE1	1:A:286:TRP:HZ3	2.32	0.47
1:C:156:ILE:HD11	1:C:162:PHE:CD2	2.49	0.47
1:A:162:PHE:HE1	1:A:286:TRP:HZ3	1.62	0.46
1:C:28:ARG:HD3	4:C:613:HOH:O	2.15	0.45
1:C:21:LEU:HD22	1:C:28:ARG:HD2	1.98	0.45
1:C:177:ILE:HD13	1:C:244:LEU:HG	1.99	0.45
1:A:161:GLU:HB3	1:A:208:VAL:CG1	2.47	0.45
1:B:269:ILE:CG2	1:B:271:GLN:HG2	2.46	0.44
1:B:310:CYS:HB2	1:B:318:ARG:NH1	2.31	0.44
1:B:14:GLU:HG2	1:B:15:LYS:CD	2.46	0.44
1:C:156:ILE:HD11	1:C:162:PHE:CD1	2.52	0.44
1:C:117:SER:HB3	1:C:118:PRO:HD3	2.00	0.44
1:B:227:LEU:HD12	1:B:231:ASP:HB3	2.00	0.44
1:B:176:GLU:HB2	1:B:213:HIS:HD2	1.83	0.44
1:C:152:GLY:O	1:C:156:ILE:HG23	2.18	0.43
1:C:48:GLU:HB3	1:C:52:SER:OG	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:NH1	1:A:233:ASP:OD1	2.41	0.43
1:B:90:LEU:HD13	1:B:260:ASP:HB3	2.01	0.43
1:A:137:LEU:HA	1:A:276:ILE:O	2.19	0.43
1:B:334:ARG:HG2	1:B:334:ARG:O	2.19	0.43
1:B:96:ASN:O	1:B:100:VAL:HG23	2.19	0.42
1:B:88:ARG:NH1	1:C:260:ASP:OD1	2.45	0.42
1:B:269:ILE:HG23	1:B:271:GLN:HG2	2.01	0.42
1:C:129:ASP:N	1:C:129:ASP:OD2	2.46	0.42
1:B:112:GLY:HA3	1:B:116:GLY:O	2.20	0.42
1:B:134:VAL:O	1:B:273:SER:HA	2.20	0.42
1:B:90:LEU:HD21	1:C:90:LEU:HD21	2.01	0.42
1:C:159:ASP:CG	1:C:160:GLU:N	2.72	0.42
1:A:250:ARG:CA	1:A:250:ARG:HE	2.31	0.42
1:C:134:VAL:O	1:C:273:SER:HA	2.20	0.42
1:B:302:SER:HB3	4:B:622:HOH:O	2.20	0.41
1:C:65:TYR:CZ	1:C:330:LEU:HB3	2.54	0.41
1:A:177:ILE:HG12	1:A:184:TRP:CE2	2.56	0.41
1:C:282:ALA:HA	1:C:285:THR:HG22	2.03	0.41
1:C:56:GLN:HG3	1:C:323:ASN:OD1	2.21	0.41
1:A:155:ARG:NH1	1:A:155:ARG:HG3	2.35	0.41
1:C:334:ARG:HG3	1:C:334:ARG:O	2.20	0.41
1:A:155:ARG:HG2	1:A:155:ARG:H	1.59	0.41
1:B:137:LEU:HA	1:B:276:ILE:O	2.22	0.40
1:A:46:PHE:HA	1:A:47:PRO:HA	1.86	0.40
1:B:17:ALA:HB1	1:B:32:VAL:CG1	2.52	0.40
1:B:227:LEU:HD12	1:B:231:ASP:CB	2.52	0.40
1:A:74:GLY:CA	1:A:80:LYS:HG2	2.47	0.40
1:B:73:ARG:CZ	1:B:91:ALA:HB1	2.51	0.40
1:C:189:TYR:HA	1:C:313:TRP:CZ2	2.56	0.40
1:C:227:LEU:HD12	1:C:231:ASP:HB3	2.03	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
4:B:671:HOH:O	4:C:645:HOH:O[3_555]	1.87	0.33

## 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	327/353 (93%)	318 (97%)	7 (2%)	2 (1%)	25	25
1	B	320/353 (91%)	314 (98%)	5 (2%)	1 (0%)	41	45
1	C	319/353 (90%)	307 (96%)	8 (2%)	4 (1%)	12	9
All	All	966/1059 (91%)	939 (97%)	20 (2%)	7 (1%)	22	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	200	GLU
1	A	159	ASP
1	C	155	ARG
1	C	159	ASP
1	B	47	PRO
1	C	47	PRO
1	A	47	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	250/269 (93%)	247 (99%)	3 (1%)	71	82
1	B	241/269 (90%)	240 (100%)	1 (0%)	91	95
1	C	240/269 (89%)	239 (100%)	1 (0%)	91	95
All	All	731/807 (91%)	726 (99%)	5 (1%)	84	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	ASP
1	A	200	GLU
1	A	250	ARG
1	B	250	ARG
1	C	159	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN

### 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](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	$\# Z  > 2$
2	CAC	A	401	-	0,4,4	0.00	-	0,6,6	0.00	-
2	CAC	B	401	-	0,4,4	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CAC	C	401	-	0,4,4	0.00	-	0,6,6	0.00	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	CAC	1	0
2	C	401	CAC	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

### 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	331/353 (93%)	-0.09	17 (5%) 28 26	24, 35, 65, 114	0
1	B	322/353 (91%)	-0.19	5 (1%) 72 70	24, 36, 54, 102	0
1	C	320/353 (90%)	-0.11	14 (4%) 34 32	28, 41, 64, 122	0
All	All	973/1059 (91%)	-0.13	36 (3%) 41 39	24, 37, 62, 122	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	335	ASN	6.4
1	C	159	ASP	6.1
1	A	159	ASP	5.8
1	C	155	ARG	4.9
1	A	204	ARG	4.2
1	A	157	GLY	3.8
1	A	155	ARG	3.7
1	A	158	GLY	3.7
1	C	104	GLY	3.6
1	C	334	ARG	3.4
1	A	353	HIS	3.3
1	A	200	GLU	3.3
1	A	346	LEU	3.1
1	C	158	GLY	3.1
1	C	286	TRP	3.0
1	B	154	ALA	2.7
1	A	211	GLY	2.7
1	A	16	GLY	2.7
1	C	333	LEU	2.6
1	A	210	PRO	2.6
1	A	220	THR	2.6
1	C	156	ILE	2.4
1	B	15	LYS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	36	THR	2.4
1	B	334	ARG	2.3
1	C	146	GLU	2.3
1	C	285	THR	2.2
1	B	159	ASP	2.2
1	A	156	ILE	2.2
1	C	295	PRO	2.2
1	C	38	PRO	2.2
1	A	209	PRO	2.2
1	A	221	GLY	2.1
1	A	284	THR	2.1
1	A	292	ASP	2.1
1	B	14	GLU	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CAC	B	401	5/5	0.91	0.19	74,75,85,107	0
3	CL	A	404	1/1	0.92	0.20	50,50,50,50	0
3	CL	B	402	1/1	0.93	0.19	52,52,52,52	0
2	CAC	A	401	5/5	0.97	0.16	50,52,54,76	0
3	CL	C	402	1/1	0.98	0.22	55,55,55,55	0
3	CL	A	403	1/1	0.99	0.18	53,53,53,53	0
2	CAC	C	401	5/5	0.99	0.09	41,45,52,71	0
3	CL	A	402	1/1	0.99	0.15	44,44,44,44	0



## 6.5 Other polymers

There are no such residues in this entry.