



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 07:29 pm GMT

PDB ID : 4J5J  
Title : Crystal Structure of Multidrug Resistant HIV-1 Protease Clinical Isolate PR20  
in Complex with Amprenavir  
Authors : Shen, C.H.; Weber, I.T.  
Deposited on : 2013-02-08  
Resolution : 1.80 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

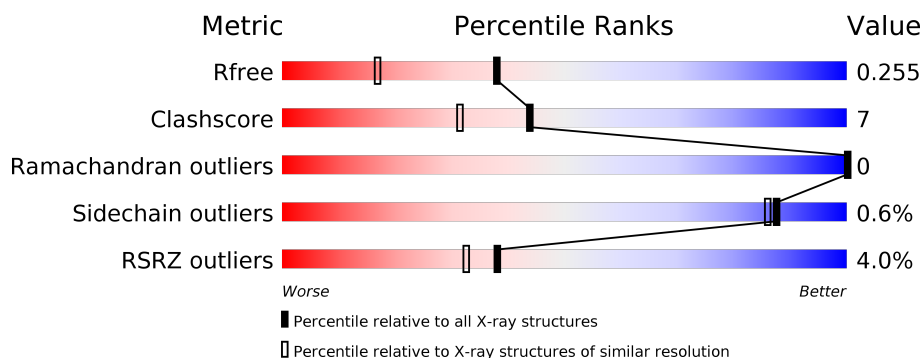
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

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. 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	99	<div> <div>4%</div> <div>80%</div> <div>19%</div> </div>
1	B	99	<div> <div>4%</div> <div>85%</div> <div>15%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1710 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 Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	3	0
			777	506	133	136	2			
1	B	99	Total	C	N	O	S	0	1	0
			765	496	131	136	2			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	GLN	ENGINEERED MUTATION	UNP P03367
A	10	PHE	LEU	ENGINEERED MUTATION	UNP P03367
A	13	VAL	ILE	ENGINEERED MUTATION	UNP P03367
A	15	VAL	ILE	ENGINEERED MUTATION	UNP P03367
A	30	ASN	ASP	ENGINEERED MUTATION	UNP P03367
A	32	ILE	VAL	ENGINEERED MUTATION	UNP P03367
A	33	PHE	LEU	ENGINEERED MUTATION	UNP P03367
A	35	ASP	GLU	ENGINEERED MUTATION	UNP P03367
A	36	ILE	MET	ENGINEERED MUTATION	UNP P03367
A	37	ASN	SER	ENGINEERED MUTATION	UNP P03367
A	47	VAL	ILE	ENGINEERED MUTATION	UNP P03367
A	54	LEU	ILE	ENGINEERED MUTATION	UNP P03367
A	58	GLU	GLN	ENGINEERED MUTATION	UNP P03367
A	62	VAL	ILE	ENGINEERED MUTATION	UNP P03367
A	63	PRO	LEU	ENGINEERED MUTATION	UNP P03367
A	67	ALA	CYS	ENGINEERED MUTATION	UNP P03367
A	71	VAL	ALA	ENGINEERED MUTATION	UNP P03367
A	84	VAL	ILE	ENGINEERED MUTATION	UNP P03367
A	88	ASP	ASN	ENGINEERED MUTATION	UNP P03367
A	89	THR	LEU	ENGINEERED MUTATION	UNP P03367
A	90	MET	LEU	ENGINEERED MUTATION	UNP P03367
A	95	ALA	CYS	ENGINEERED MUTATION	UNP P03367
B	107	LYS	GLN	ENGINEERED MUTATION	UNP P03367
B	110	PHE	LEU	ENGINEERED MUTATION	UNP P03367
B	113	VAL	ILE	ENGINEERED MUTATION	UNP P03367

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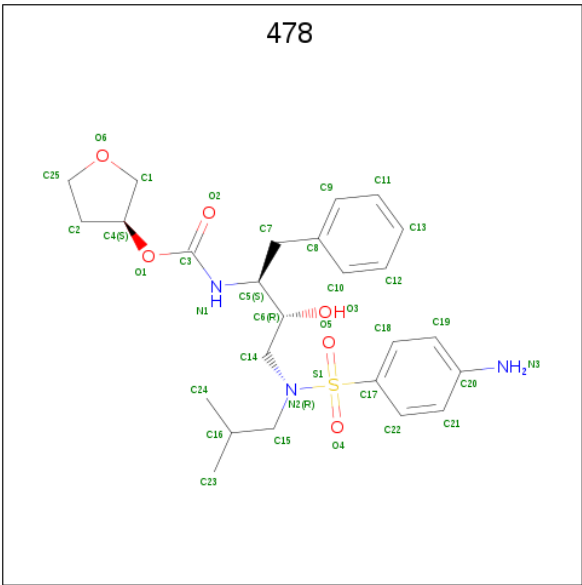
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Chain	Residue	Modelled	Actual	Comment	Reference
B	115	VAL	ILE	ENGINEERED MUTATION	UNP P03367
B	130	ASN	ASP	ENGINEERED MUTATION	UNP P03367
B	132	ILE	VAL	ENGINEERED MUTATION	UNP P03367
B	133	PHE	LEU	ENGINEERED MUTATION	UNP P03367
B	135	ASP	GLU	ENGINEERED MUTATION	UNP P03367
B	136	ILE	MET	ENGINEERED MUTATION	UNP P03367
B	137	ASN	SER	ENGINEERED MUTATION	UNP P03367
B	147	VAL	ILE	ENGINEERED MUTATION	UNP P03367
B	154	LEU	ILE	ENGINEERED MUTATION	UNP P03367
B	158	GLU	GLN	ENGINEERED MUTATION	UNP P03367
B	162	VAL	ILE	ENGINEERED MUTATION	UNP P03367
B	163	PRO	LEU	ENGINEERED MUTATION	UNP P03367
B	167	ALA	CYS	ENGINEERED MUTATION	UNP P03367
B	171	VAL	ALA	ENGINEERED MUTATION	UNP P03367
B	184	VAL	ILE	ENGINEERED MUTATION	UNP P03367
B	188	ASP	ASN	ENGINEERED MUTATION	UNP P03367
B	189	THR	LEU	ENGINEERED MUTATION	UNP P03367
B	190	MET	LEU	ENGINEERED MUTATION	UNP P03367
B	195	ALA	CYS	ENGINEERED MUTATION	UNP P03367

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Cl 2 2	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is {3-[(4-AMINO-BENZENESULFONYL)-ISOBUTYL-AMINO]-1-BENZYL-2-HYDROXY-PROPYL}-CARBAMIC ACID TETRAHYDRO-FURAN-3-YL ESTER (three-letter code: 478) (formula: C<sub>25</sub>H<sub>35</sub>N<sub>3</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			35	25	3	6	1		
3	B	1	Total	C	N	O	S	0	0
			35	25	3	6	1		

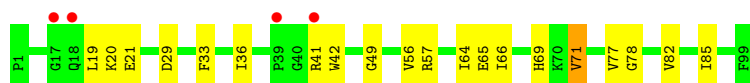
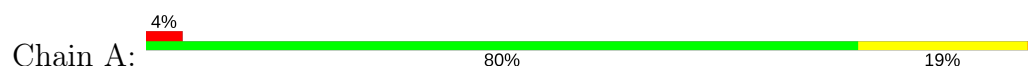
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	51	Total	O	0	0
			51	51		

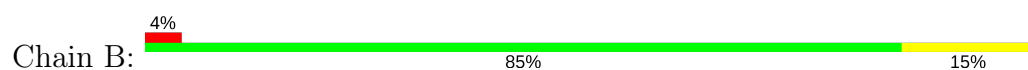
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Protease



#### ● Molecule 1: Protease



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	28.72Å 65.80Å 93.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.91 – 1.80 9.91 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (9.91-1.80) 97.7 (9.91-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.187 , 0.243 0.198 , 0.255	Depositor DCC
$R_{free}$ test set	828 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1710	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 10.86% 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: 478, 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	1.10	1/802 (0.1%)	1.05	3/1087 (0.3%)
1	B	1.10	0/784	0.95	1/1062 (0.1%)
All	All	1.10	1/1586 (0.1%)	1.00	4/2149 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	GLU	CB-CG	-8.53	1.35	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ASP	CB-CG-OD1	8.62	126.06	118.30
1	B	108	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	A	29	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	A	71	VAL	CG1-CB-CG2	-5.17	102.63	110.90

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	777	0	827	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	765	0	803	12	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	B	70	0	70	3	0
4	A	44	0	0	1	0
4	B	51	0	0	1	0
All	All	1710	0	1700	24	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 7.

All (24) 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:57[B]:ARG:NH2	4:A:543:HOH:O	1.62	1.24
1:B:170:LYS:HE2	1:B:172:ILE:HD11	1.48	0.94
3:B:402:478:H5	3:B:402:478:H152	1.62	0.79
1:A:49:GLY:HA3	1:B:150:ILE:HB	1.73	0.70
1:A:56:VAL:HG12	1:A:78:GLY:HA3	1.77	0.67
1:A:64:ILE:HB	1:A:71:VAL:HG22	1.84	0.59
1:B:120:LYS:NZ	1:B:136:ILE:HG22	2.18	0.58
1:A:20:LYS:HE3	1:A:36:ILE:HG22	1.85	0.57
1:B:134:GLU:HG2	1:B:183:ASN:OD1	2.04	0.56
3:B:402:478:H243	3:B:402:478:H10	1.88	0.56
1:B:163:PRO:HB3	1:B:170:LYS:HE3	1.88	0.55
1:A:65:GLU:HA	1:A:69:HIS:O	2.08	0.53
1:B:120:LYS:HZ1	1:B:136:ILE:HG22	1.72	0.53
1:A:66:ILE:HD13	1:A:85[B]:ILE:HD13	1.92	0.51
1:A:33:PHE:O	1:A:77:VAL:HA	2.13	0.48
1:B:141:ARG:HD3	4:B:550:HOH:O	2.13	0.48
1:B:154:LEU:HD11	1:B:179:PRO:HD2	1.96	0.47
1:B:120:LYS:NZ	1:B:136:ILE:CG2	2.78	0.46
1:A:82:VAL:HG11	3:B:401:478:H241	1.98	0.44
1:A:41:ARG:HG2	1:A:42:TRP:H	1.83	0.44
1:B:167:ALA:HB3	1:B:169:HIS:CD2	2.53	0.43
1:A:57[B]:ARG:HG2	1:A:77:VAL:O	2.18	0.43
1:B:120:LYS:HZ2	1:B:136:ILE:CG2	2.34	0.41
1:B:114:LYS:HB2	1:B:114:LYS:HE3	1.88	0.40

There are no symmetry-related clashes.

## 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	100/99 (101%)	99 (99%)	1 (1%)	0	100	100
1	B	98/99 (99%)	94 (96%)	4 (4%)	0	100	100
All	All	198/198 (100%)	193 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	85/82 (104%)	84 (99%)	1 (1%)	74	68
1	B	83/82 (101%)	83 (100%)	0	100	100
All	All	168/164 (102%)	167 (99%)	1 (1%)	87	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	98	ASN

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Mol	Chain	Res	Type
1	B	161	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z  > 2$
3	478	B	401	-	37,37,37	1.80	5 (13%)	47,51,51	2.03	14 (29%)
3	478	B	402	-	37,37,37	2.20	3 (8%)	47,51,51	2.60	12 (25%)

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	478	B	401	-	-	0/36/43/43	0/3/3/3
3	478	B	402	-	-	0/36/43/43	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	478	C17-S1	-10.32	1.61	1.76
3	B	401	478	C17-S1	-7.25	1.66	1.76
3	B	401	478	O5-S1	-2.35	1.40	1.43
3	B	401	478	C18-C17	2.06	1.42	1.38
3	B	401	478	C19-C18	2.12	1.42	1.38
3	B	402	478	C14-N2	2.62	1.52	1.47
3	B	401	478	O1-C3	5.22	1.44	1.35
3	B	402	478	O1-C3	6.31	1.46	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	478	C17-S1-N2	-8.03	97.59	107.30
3	B	402	478	O5-S1-O4	-6.77	108.37	119.50
3	B	401	478	O5-S1-N2	-5.92	101.19	106.69
3	B	401	478	O5-S1-O4	-3.86	113.16	119.50
3	B	401	478	C22-C17-C18	-3.49	115.46	120.43
3	B	402	478	O1-C3-O2	-3.47	119.32	124.51
3	B	401	478	C14-N2-S1	-3.35	110.32	117.64
3	B	401	478	C7-C5-N1	-3.16	106.59	110.21
3	B	402	478	C8-C7-C5	-2.74	108.49	113.36
3	B	401	478	C4-O1-C3	-2.70	112.58	116.48
3	B	401	478	O1-C3-O2	-2.52	120.73	124.51
3	B	402	478	C18-C17-S1	-2.35	117.27	119.77
3	B	402	478	C7-C5-N1	-2.10	107.81	110.21
3	B	402	478	O5-S1-N2	2.12	108.66	106.69
3	B	401	478	O1-C3-N1	2.18	113.13	110.40
3	B	402	478	C25-C2-C4	2.80	105.70	102.77
3	B	401	478	C19-C18-C17	2.89	122.51	119.46
3	B	401	478	C17-S1-N2	2.91	110.82	107.30
3	B	401	478	C21-C22-C17	2.93	122.56	119.46
3	B	401	478	C22-C17-S1	3.46	123.46	119.77
3	B	401	478	O5-S1-C17	3.64	112.69	108.02
3	B	402	478	C22-C17-S1	3.86	123.89	119.77
3	B	401	478	O4-S1-N2	4.03	110.43	106.69
3	B	402	478	O1-C3-N1	5.89	117.79	110.40
3	B	402	478	O5-S1-C17	6.46	116.32	108.02
3	B	402	478	O4-S1-C17	6.64	116.54	108.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	478	1	0
3	B	402	478	2	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	99/99 (100%)	0.05	4 (4%) 38 32	11, 24, 46, 60	0
1	B	99/99 (100%)	-0.07	4 (4%) 38 32	11, 22, 40, 46	0
All	All	198/198 (100%)	-0.01	8 (4%) 38 32	11, 22, 43, 60	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	ASN	3.7
1	B	139	PRO	3.6
1	A	39	PRO	3.1
1	A	41	ARG	2.9
1	B	135	ASP	2.6
1	B	168	GLY	2.4
1	A	18	GLN	2.1
1	A	17	GLY	2.0

### 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 carbohydrates 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(Å <sup>2</sup> )	Q<0.9
3	478	B	402	35/35	0.85	0.20	19,41,50,52	35
2	CL	B	404	1/1	0.92	0.20	25,25,25,25	1
2	CL	A	101	1/1	0.94	0.14	30,30,30,30	1
2	CL	B	403	1/1	0.95	0.14	36,36,36,36	0
3	478	B	401	35/35	0.97	0.07	13,20,25,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.