



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2017 – 02:30 PM EDT

PDB ID : 1DVM  
Title : ACTIVE FORM OF HUMAN PAI-1  
Authors : Stout, T.J.; Graham, H.; Buckley, D.I.; Matthews, D.J.  
Deposited on : unknown  
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

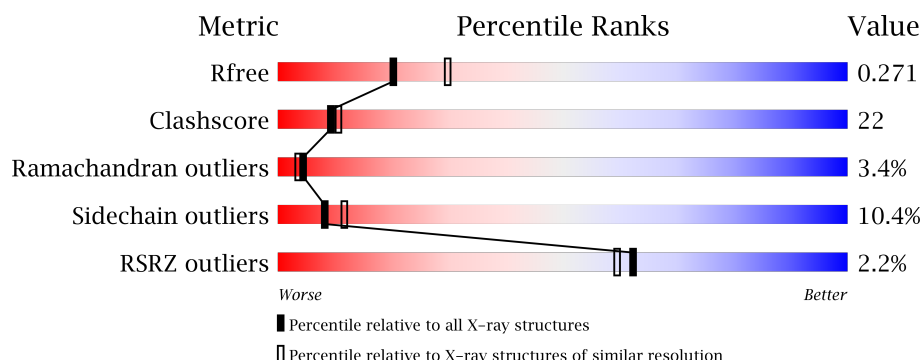
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	379	<div> <div>2%</div> <div>56%</div> <div>39%</div> <div>...</div> </div>
1	B	379	<div> <div>2%</div> <div>54%</div> <div>36%</div> <div>6%</div> <div>...</div> </div>
1	C	379	<div> <div>2%</div> <div>51%</div> <div>36%</div> <div>7%</div> <div>...</div> </div>
1	D	379	<div> <div>2%</div> <div>54%</div> <div>36%</div> <div>7%</div> <div>...</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria.

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	1001	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13383 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 PLASMINOGEN ACTIVATOR INHIBITOR-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2973	1909	505	544	15			
1	B	365	Total	C	N	O	S	0	0	0
			2912	1872	495	530	15			
1	C	364	Total	C	N	O	S	11	0	0
			2902	1864	494	529	15			
1	D	372	Total	C	N	O	S	0	0	0
			2956	1899	502	540	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	HIS	ASN	ENGINEERED	UNP P05121
A	154	THR	LYS	ENGINEERED	UNP P05121
A	319	LEU	GLN	ENGINEERED	UNP P05121
A	354	ILE	MET	ENGINEERED	UNP P05121
B	150	HIS	ASN	ENGINEERED	UNP P05121
B	154	THR	LYS	ENGINEERED	UNP P05121
B	319	LEU	GLN	ENGINEERED	UNP P05121
B	354	ILE	MET	ENGINEERED	UNP P05121
C	150	HIS	ASN	ENGINEERED	UNP P05121
C	154	THR	LYS	ENGINEERED	UNP P05121
C	319	LEU	GLN	ENGINEERED	UNP P05121
C	354	ILE	MET	ENGINEERED	UNP P05121
D	150	HIS	ASN	ENGINEERED	UNP P05121
D	154	THR	LYS	ENGINEERED	UNP P05121
D	319	LEU	GLN	ENGINEERED	UNP P05121
D	354	ILE	MET	ENGINEERED	UNP P05121

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

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

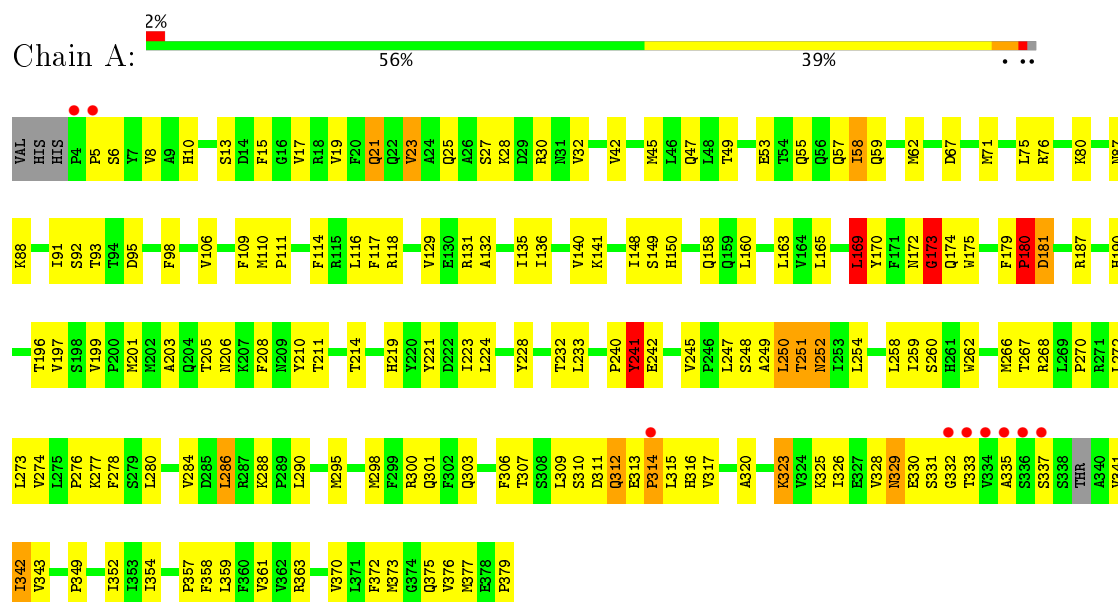
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	434	Total O 434 434	0	0
3	B	398	Total O 398 398	0	0
3	C	352	Total O 352 352	0	0
3	D	452	Total O 452 452	0	0

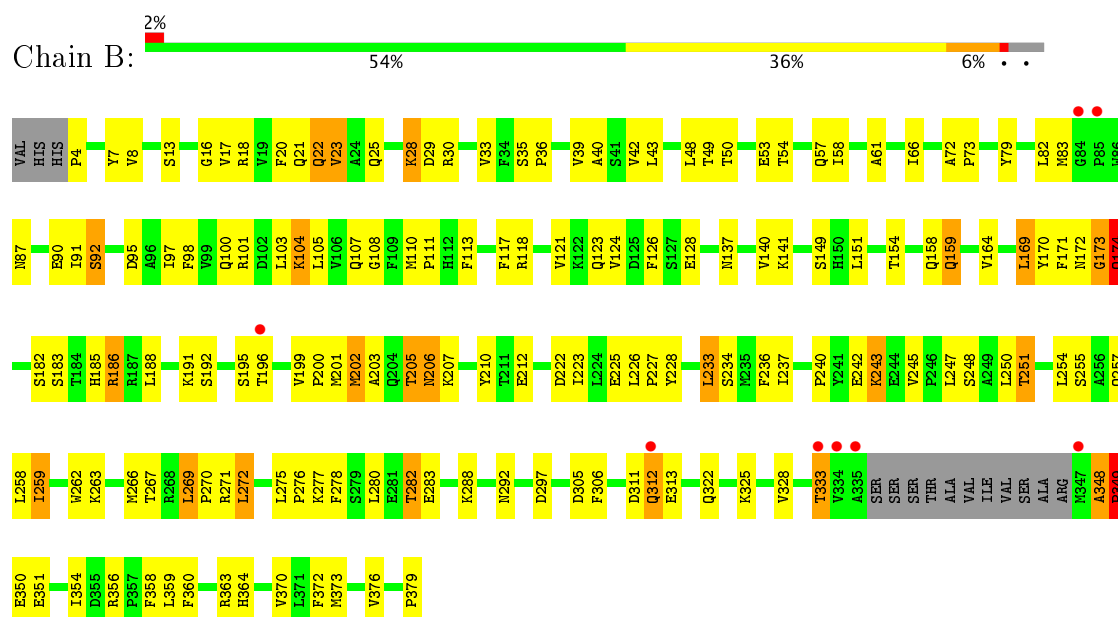
### 3 Residue-property plots

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

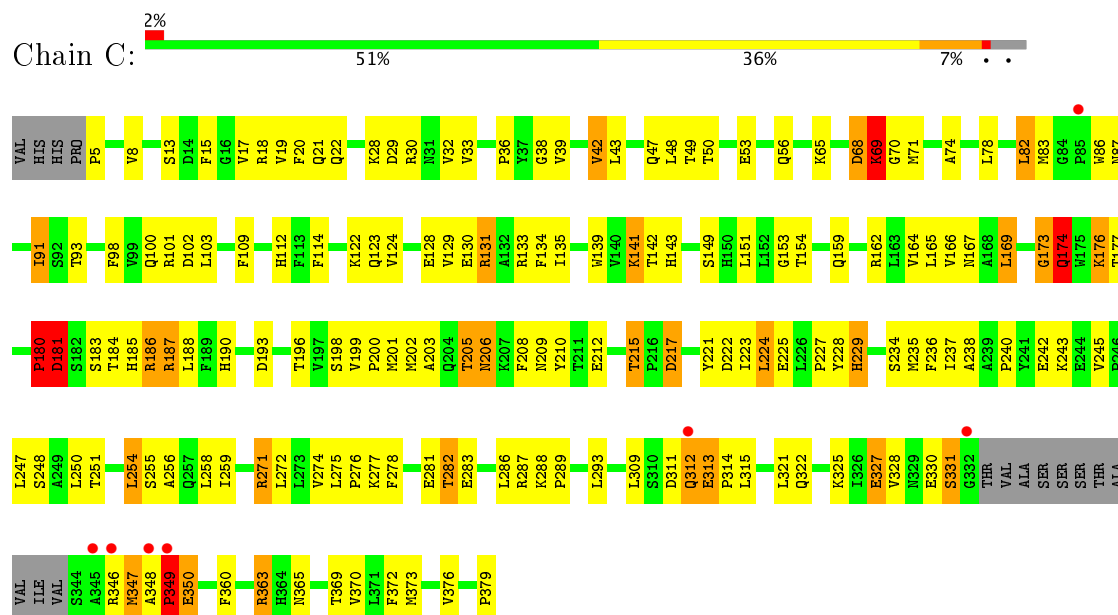
#### • Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1



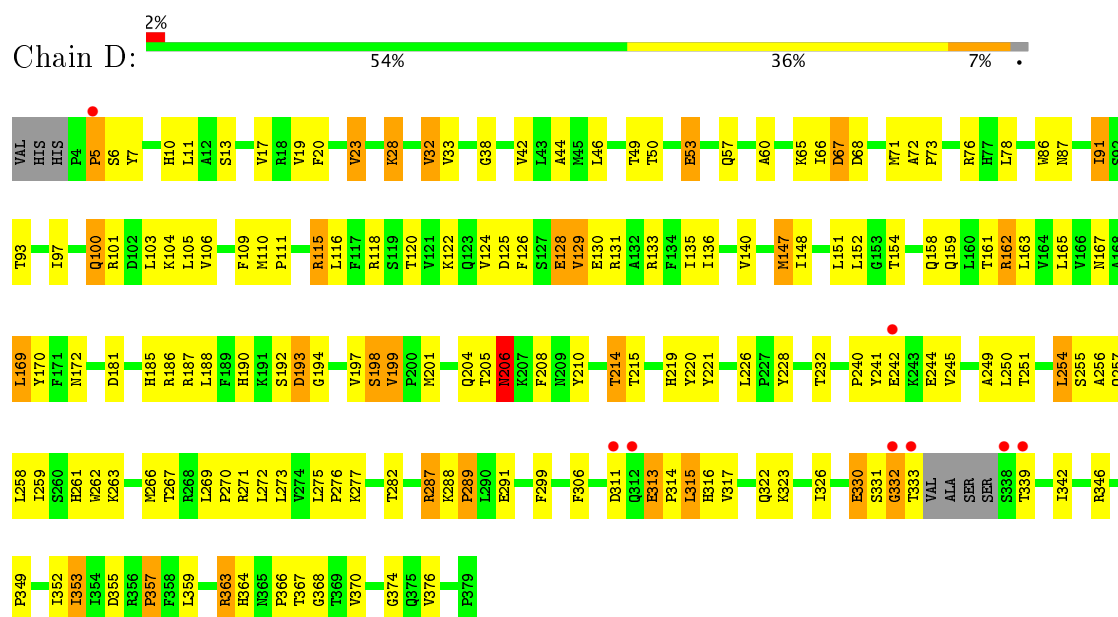
#### • Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1



• Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1



• Molecule 1: PLASMINOGEN ACTIVATOR INHIBITOR-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.76Å 74.67Å 103.44Å 85.19° 86.17° 64.34°	Depositor
Resolution (Å)	30.00 – 2.40 25.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	80.5 (30.00-2.40) 79.2 (25.76-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 98.0	Depositor
R, $R_{free}$	0.218 , 0.292 0.188 , 0.271	Depositor DCC
$R_{free}$ test set	2194 reflections (4.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 101.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13383	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 5.84% 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: 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	0.45	2/3045 (0.1%)	0.74	3/4129 (0.1%)
1	B	0.41	0/2984	0.70	1/4045 (0.0%)
1	C	0.41	0/2973	0.71	1/4028 (0.0%)
1	D	0.44	0/3028	0.73	0/4106
All	All	0.43	2/12030 (0.0%)	0.72	5/16308 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	TYR	CD2-CE2	-6.08	1.30	1.39
1	A	241	TYR	CE2-CZ	-5.53	1.31	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	GLY	N-CA-C	6.66	129.74	113.10
1	A	169	LEU	CA-CB-CG	5.90	128.87	115.30
1	A	332	GLY	N-CA-C	-5.85	98.48	113.10
1	B	233	LEU	CA-CB-CG	5.33	127.57	115.30
1	C	350	GLU	N-CA-C	5.17	124.95	111.00

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	2973	0	2967	116	0
1	B	2912	0	2906	136	0
1	C	2902	0	2890	131	0
1	D	2956	0	2950	142	0
2	A	1	0	0	2	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	434	0	0	7	0
3	B	398	0	0	6	0
3	C	352	0	0	8	0
3	D	452	0	0	10	0
All	All	13383	0	11713	516	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 22.

The worst 5 of 516 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:C:271:ARG:HH11	1:C:271:ARG:HG2	1.14	1.08
1:B:243:LYS:H	1:B:243:LYS:HD3	1.17	1.06
1:B:104:LYS:H	1:B:104:LYS:HD2	1.19	1.05
1:D:162:ARG:HG2	1:D:162:ARG:HH11	1.24	0.98
1:A:254:LEU:HD23	1:A:373:MET:HE3	1.43	0.97

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	371/379 (98%)	330 (89%)	28 (8%)	13 (4%)	4	3
1	B	361/379 (95%)	333 (92%)	20 (6%)	8 (2%)	8	9
1	C	360/379 (95%)	325 (90%)	22 (6%)	13 (4%)	4	3
1	D	368/379 (97%)	326 (89%)	27 (7%)	15 (4%)	3	2
All	All	1460/1516 (96%)	1314 (90%)	97 (7%)	49 (3%)	4	3

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	173	GLY
1	A	174	GLN
1	A	180	PRO
1	A	181	ASP

### 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	328/333 (98%)	300 (92%)	28 (8%)	12	19
1	B	321/333 (96%)	290 (90%)	31 (10%)	9	14
1	C	319/333 (96%)	281 (88%)	38 (12%)	6	8
1	D	326/333 (98%)	289 (89%)	37 (11%)	7	9
All	All	1294/1332 (97%)	1160 (90%)	134 (10%)	8	12

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	42	VAL
1	C	198	SER
1	D	250	LEU
1	C	82	LEU
1	C	162	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	312	GLN
1	C	143	HIS
1	D	174	GLN
1	C	22	GLN
1	C	87	ASN

### 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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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	375/379 (98%)	-0.53	9 (2%) 59 56	3, 16, 45, 80	2 (0%)
1	B	365/379 (96%)	-0.38	8 (2%) 62 59	5, 20, 51, 92	0
1	C	364/379 (96%)	-0.36	7 (1%) 67 64	4, 21, 49, 82	2 (0%)
1	D	372/379 (98%)	-0.53	8 (2%) 62 59	3, 17, 42, 82	0
All	All	1476/1516 (97%)	-0.45	32 (2%) 62 59	3, 19, 48, 92	4 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	333	THR	6.3
1	A	336	SER	6.2
1	A	5	PRO	5.9
1	B	333	THR	5.7
1	B	335	ALA	5.5

### 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	1001	1/1	0.99	0.12	0.79	24,24,24,24	0
2	CL	B	1004	1/1	0.99	0.11	-0.19	32,32,32,32	0
2	CL	C	1003	1/1	0.99	0.05	-4.04	26,26,26,26	0
2	CL	D	1002	1/1	0.98	0.06	-9.30	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.