



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 09:03 AM UTC

PDB ID : 2PNL / pdb_00002pnl
Title : Crystal structure of VP4 protease from infectious pancreatic necrosis virus (IPNV) in space group P1
Authors : Paetzel, M.; Lee, J.; Feldman, A.R.; Delmas, B.
Deposited on : 2007-04-24
Resolution : 2.21 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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

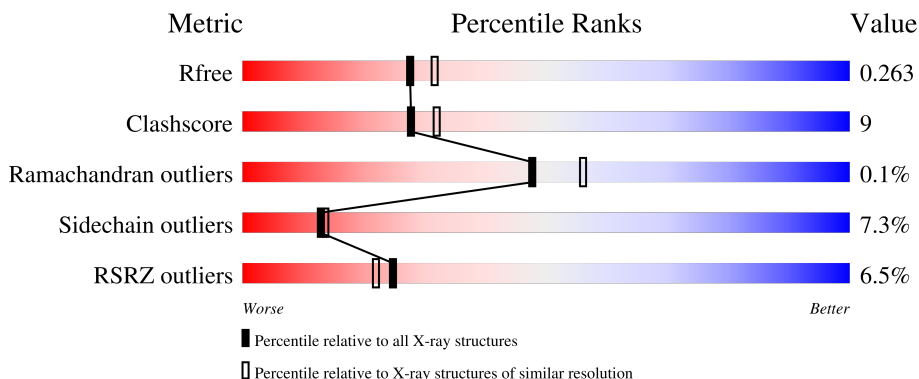
1 Overall quality at a glance

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.



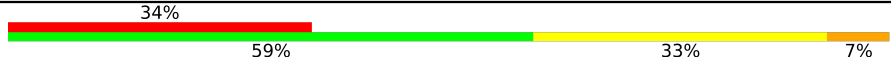




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	203	 81% 18% .
1	B	203	 83% 16% .
1	C	203	 83% 16% .
1	D	203	 % 77% 20% .
1	E	203	 80% 18% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	203	 34% 59% 33% 7%
1	G	203	 27% 69% 23% 7%
1	H	203	 77% 22%
1	I	203	 81% 17% •
1	J	203	 86% 12% ••

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16426 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 VP4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	203	1509	957	250	297	2	3	0	0	0
1	B	203	1515	960	253	297	2	3	0	0	0
1	C	203	1515	960	253	297	2	3	0	0	0
1	D	203	1515	960	253	297	2	3	0	0	0
1	E	203	1519	963	254	297	2	3	0	0	0
1	F	203	1513	960	251	297	2	3	0	0	0
1	G	203	1515	960	253	297	2	3	0	0	0
1	H	203	1516	960	253	298	2	3	0	0	0
1	I	203	1516	960	253	298	2	3	0	0	0
1	J	203	1509	957	250	297	2	3	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

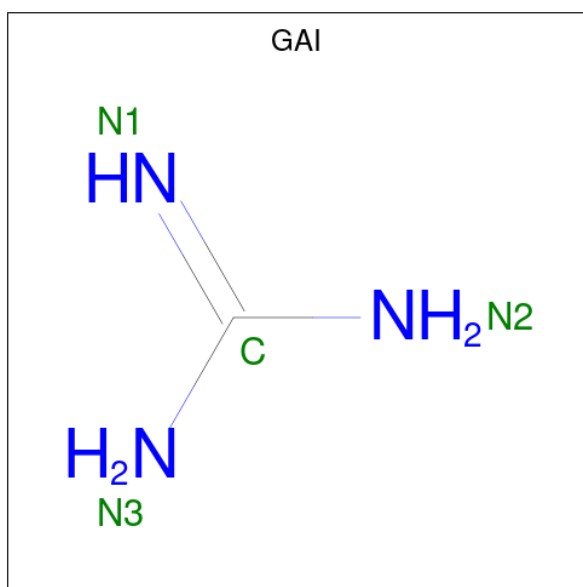
Chain	Residue	Modelled	Actual	Comment	Reference
A	603	MSE	MET	modified residue	UNP Q703G9
A	630	MSE	MET	modified residue	UNP Q703G9
A	652	MSE	MET	modified residue	UNP Q703G9
A	674	ALA	LYS	engineered mutation	UNP Q703G9
B	603	MSE	MET	modified residue	UNP Q703G9
B	630	MSE	MET	modified residue	UNP Q703G9
B	652	MSE	MET	modified residue	UNP Q703G9
B	674	ALA	LYS	engineered mutation	UNP Q703G9
C	603	MSE	MET	modified residue	UNP Q703G9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	630	MSE	MET	modified residue	UNP Q703G9
C	652	MSE	MET	modified residue	UNP Q703G9
C	674	ALA	LYS	engineered mutation	UNP Q703G9
D	603	MSE	MET	modified residue	UNP Q703G9
D	630	MSE	MET	modified residue	UNP Q703G9
D	652	MSE	MET	modified residue	UNP Q703G9
D	674	ALA	LYS	engineered mutation	UNP Q703G9
E	603	MSE	MET	modified residue	UNP Q703G9
E	630	MSE	MET	modified residue	UNP Q703G9
E	652	MSE	MET	modified residue	UNP Q703G9
E	674	ALA	LYS	engineered mutation	UNP Q703G9
F	603	MSE	MET	modified residue	UNP Q703G9
F	630	MSE	MET	modified residue	UNP Q703G9
F	652	MSE	MET	modified residue	UNP Q703G9
F	674	ALA	LYS	engineered mutation	UNP Q703G9
G	603	MSE	MET	modified residue	UNP Q703G9
G	630	MSE	MET	modified residue	UNP Q703G9
G	652	MSE	MET	modified residue	UNP Q703G9
G	674	ALA	LYS	engineered mutation	UNP Q703G9
H	603	MSE	MET	modified residue	UNP Q703G9
H	630	MSE	MET	modified residue	UNP Q703G9
H	652	MSE	MET	modified residue	UNP Q703G9
H	674	ALA	LYS	engineered mutation	UNP Q703G9
I	603	MSE	MET	modified residue	UNP Q703G9
I	630	MSE	MET	modified residue	UNP Q703G9
I	652	MSE	MET	modified residue	UNP Q703G9
I	674	ALA	LYS	engineered mutation	UNP Q703G9
J	603	MSE	MET	modified residue	UNP Q703G9
J	630	MSE	MET	modified residue	UNP Q703G9
J	652	MSE	MET	modified residue	UNP Q703G9
J	674	ALA	LYS	engineered mutation	UNP Q703G9

- Molecule 2 is GUANIDINE (CCD ID: GAI) (formula: CH₅N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			4	1	3		
2	A	1	Total	C	N	0	0
			4	1	3		
2	B	1	Total	C	N	0	0
			4	1	3		
2	B	1	Total	C	N	0	0
			4	1	3		
2	B	1	Total	C	N	0	0
			4	1	3		
2	C	1	Total	C	N	0	0
			4	1	3		
2	C	1	Total	C	N	0	0
			4	1	3		
2	C	1	Total	C	N	0	0
			4	1	3		
2	D	1	Total	C	N	0	0
			4	1	3		
2	E	1	Total	C	N	0	0
			4	1	3		
2	E	1	Total	C	N	0	0
			4	1	3		
2	F	1	Total	C	N	0	0
			4	1	3		
2	H	1	Total	C	N	0	0
			4	1	3		
2	H	1	Total	C	N	0	0
			4	1	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	N	0	0
			4	1	3		
2	I	1	Total	C	N	0	0
			4	1	3		
2	J	1	Total	C	N	0	0
			4	1	3		

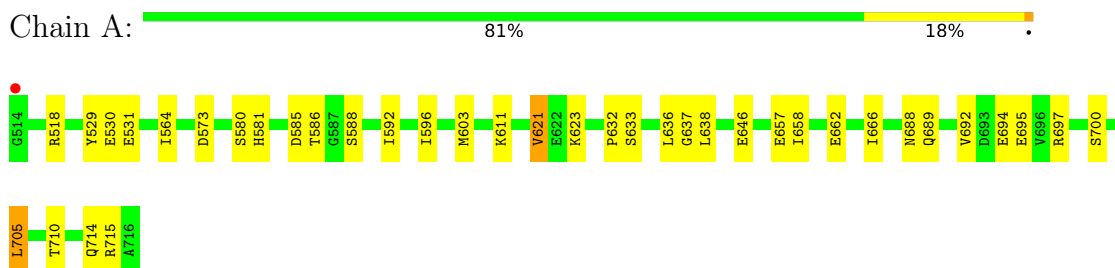
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	161	Total	O	0	0
			161	161		
3	C	141	Total	O	0	0
			141	141		
3	D	98	Total	O	0	0
			98	98		
3	E	145	Total	O	0	0
			145	145		
3	F	63	Total	O	0	0
			63	63		
3	G	66	Total	O	0	0
			66	66		
3	H	160	Total	O	0	0
			160	160		
3	I	123	Total	O	0	0
			123	123		
3	J	141	Total	O	0	0
			141	141		

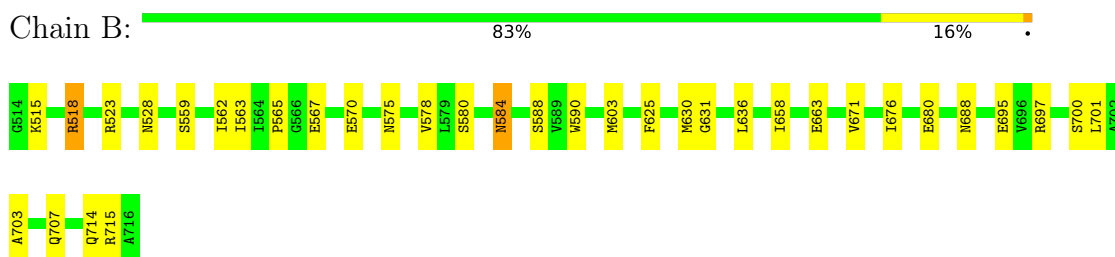
3 Residue-property plots [i](#)

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.

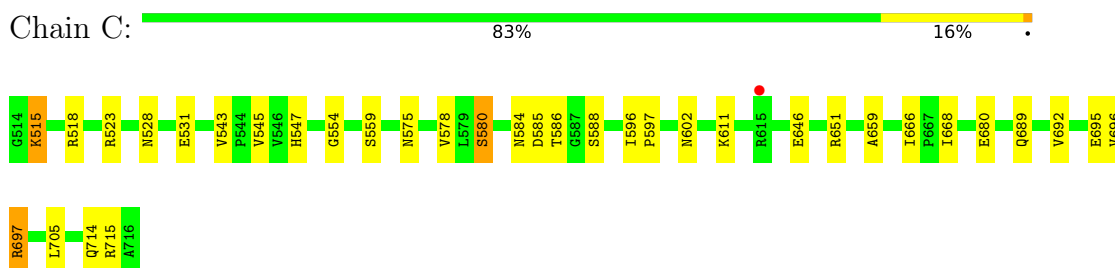
- Molecule 1: Protease VP4



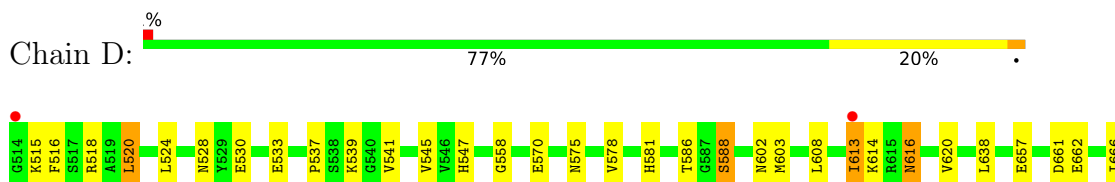
- Molecule 1: Protease VP4



- Molecule 1: Protease VP4



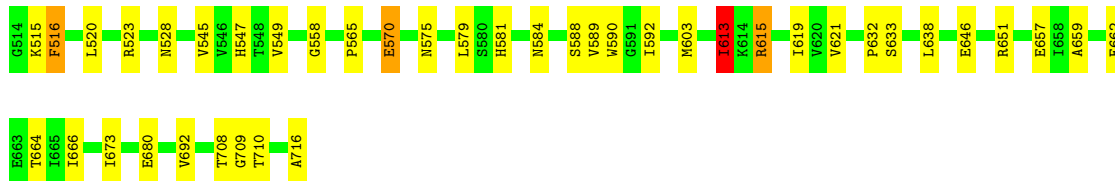
- Molecule 1: Protease VP4





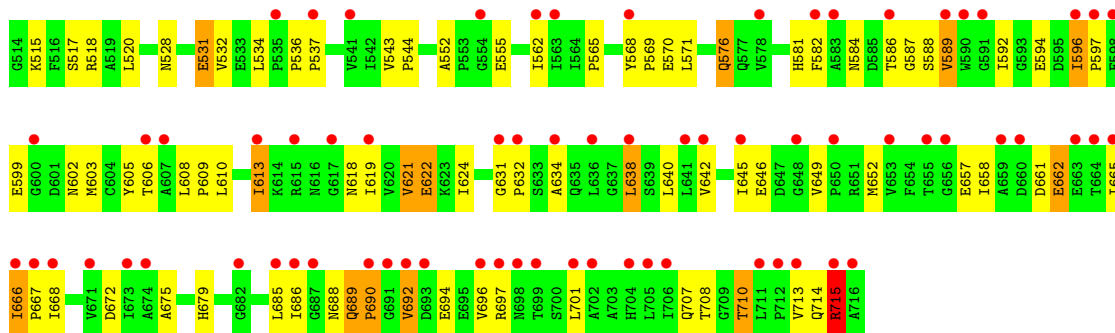
- Molecule 1: Protease VP4

Chain E: 80% 18%



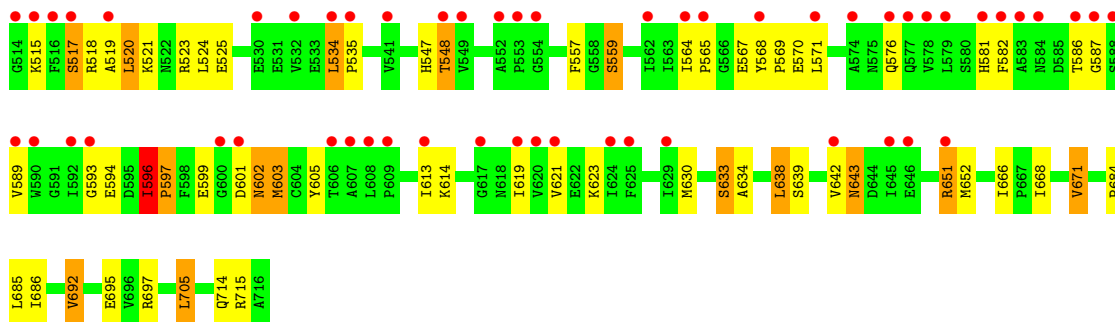
- Molecule 1: Protease VP4

Chain F: 34% 59% 33% 7%



- Molecule 1: Protease VP4

Chain G: 27% 69% 23% 7%



- Molecule 1: Protease VP4

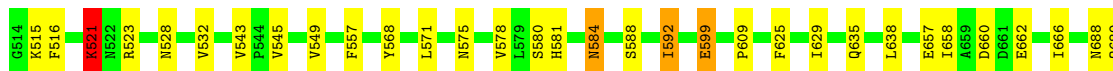
Chain H: 77% 22%





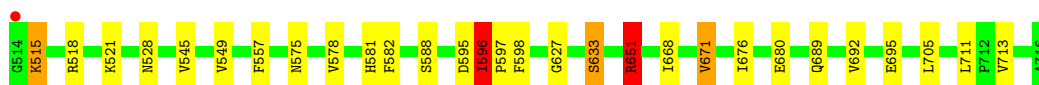
- Molecule 1: Protease VP4

Chain I: 81% 17% .



- Molecule 1: Protease VP4

Chain J: 86% 12% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.70Å 69.26Å 191.39Å 93.06° 95.03° 97.56°	Depositor
Resolution (Å)	182.57 – 2.21 182.57 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.3 (182.57-2.21) 98.2 (182.57-2.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.267 0.189 , 0.263	Depositor DCC
R_{free} test set	5185 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtrriage
Anisotropy	0.685	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16426	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GAI

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	1.15	5/1536 (0.3%)	1.10	2/2092 (0.1%)
1	B	1.16	7/1542 (0.5%)	1.13	2/2099 (0.1%)
1	C	1.07	1/1542 (0.1%)	1.14	3/2099 (0.1%)
1	D	1.07	0/1542	1.08	2/2099 (0.1%)
1	E	1.16	4/1546 (0.3%)	1.16	4/2103 (0.2%)
1	F	0.94	1/1540 (0.1%)	1.13	6/2096 (0.3%)
1	G	1.03	2/1542 (0.1%)	1.17	8/2099 (0.4%)
1	H	1.26	8/1543 (0.5%)	1.07	2/2099 (0.1%)
1	I	1.22	3/1543 (0.2%)	1.13	4/2099 (0.2%)
1	J	1.15	3/1536 (0.2%)	1.16	9/2092 (0.4%)
All	All	1.12	34/15412 (0.2%)	1.13	42/20977 (0.2%)

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
1	F	0	1
All	All	0	2

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	543	VAL	CA-CB	9.38	1.63	1.55
1	J	596	ILE	CA-CB	7.04	1.63	1.54
1	I	629	ILE	CA-CB	6.84	1.61	1.53
1	H	526	SER	C-O	-6.83	1.15	1.24
1	I	599	GLU	C-O	-6.73	1.15	1.23

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	584	ASN	CA-C-N	-11.88	103.88	123.37
1	E	584	ASN	C-N-CA	-11.88	103.88	123.37
1	C	584	ASN	CA-C-N	-10.55	108.65	122.79
1	C	584	ASN	C-N-CA	-10.55	108.65	122.79
1	J	596	ILE	CB-CA-C	10.11	121.25	110.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	585	ASP	Peptide
1	F	715	ARG	Peptide

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	1509	0	1494	20	1
1	B	1515	0	1504	26	0
1	C	1515	0	1504	24	0
1	D	1515	0	1504	30	0
1	E	1519	0	1515	23	1
1	F	1513	0	1505	69	0
1	G	1515	0	1504	47	0
1	H	1516	0	1504	23	0
1	I	1516	0	1505	25	0
1	J	1509	0	1494	21	0
2	A	8	0	8	0	0
2	B	12	0	12	2	0
2	C	12	0	12	2	0
2	D	4	0	4	0	0
2	E	8	0	8	1	0
2	F	4	0	4	1	0
2	H	12	0	12	1	0
2	I	4	0	4	1	0
2	J	4	0	4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	118	0	0	3	0
3	B	161	0	0	4	0
3	C	141	0	0	3	0
3	D	98	0	0	3	0
3	E	145	0	0	1	0
3	F	63	0	0	4	0
3	G	66	0	0	1	0
3	H	160	0	0	3	0
3	I	123	0	0	3	0
3	J	141	0	0	1	0
All	All	16426	0	15101	272	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 9.

The worst 5 of 272 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:F:582:PHE:CD2	1:F:596:ILE:HD11	1.64	1.28
1:J:582:PHE:CD2	1:J:596:ILE:HD12	1.79	1.17
1:D:603:MSE:HG2	3:D:2101:HOH:O	1.48	1.13
1:C:715:ARG:NH2	3:C:2061:HOH:O	1.81	1.13
1:J:633:SER:HB2	1:J:668:ILE:HG21	1.41	1.02

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)
1:A:633:SER:OG	1:E:716:ALA:C[1_656]	1.99	0.21

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	201/203 (99%)	190 (94%)	11 (6%)	0	100	100
1	B	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	24	26
1	C	201/203 (99%)	195 (97%)	6 (3%)	0	100	100
1	D	201/203 (99%)	187 (93%)	14 (7%)	0	100	100
1	E	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
1	F	201/203 (99%)	185 (92%)	14 (7%)	2 (1%)	12	11
1	G	201/203 (99%)	178 (89%)	23 (11%)	0	100	100
1	H	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
1	I	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
1	J	201/203 (99%)	195 (97%)	6 (3%)	0	100	100
All	All	2010/2030 (99%)	1906 (95%)	101 (5%)	3 (0%)	48	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	584	ASN
1	F	690	PRO
1	F	584	ASN

5.3.2 Protein sidechains [i](#)

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	163/162 (101%)	157 (96%)	6 (4%)	30	39
1	B	164/162 (101%)	160 (98%)	4 (2%)	43	56
1	C	164/162 (101%)	156 (95%)	8 (5%)	22	27
1	D	164/162 (101%)	149 (91%)	15 (9%)	9	8
1	E	165/162 (102%)	154 (93%)	11 (7%)	15	16
1	F	164/162 (101%)	141 (86%)	23 (14%)	3	2
1	G	164/162 (101%)	142 (87%)	22 (13%)	4	3
1	H	164/162 (101%)	154 (94%)	10 (6%)	17	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	164/162 (101%)	155 (94%)	9 (6%)	19	23
1	J	163/162 (101%)	152 (93%)	11 (7%)	15	16
All	All	1639/1620 (101%)	1520 (93%)	119 (7%)	13	13

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	662	GLU
1	J	578	VAL
1	G	559	SER
1	J	518	ARG
1	J	713	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	581	HIS
1	I	688	ASN
1	J	602	ASN
1	D	602	ASN
1	D	581	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands are 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	GAI	H	2008	-	3,3,3	1.30	0	3,3,3	1.12	0
2	GAI	I	2012	-	3,3,3	0.88	0	3,3,3	1.01	0
2	GAI	C	2014	-	3,3,3	1.64	1 (33%)	3,3,3	1.97	1 (33%)
2	GAI	A	2002	-	3,3,3	1.06	0	3,3,3	1.13	0
2	GAI	E	2015	-	3,3,3	1.57	1 (33%)	3,3,3	0.30	0
2	GAI	H	2017	-	3,3,3	0.95	0	3,3,3	0.92	0
2	GAI	F	2011	-	3,3,3	0.91	0	3,3,3	1.19	0
2	GAI	C	2001	-	3,3,3	0.21	0	3,3,3	0.99	0
2	GAI	E	2007	-	3,3,3	0.57	0	3,3,3	0.84	0
2	GAI	B	2003	-	3,3,3	0.88	0	3,3,3	0.96	0
2	GAI	C	2006	-	3,3,3	1.44	0	3,3,3	1.51	1 (33%)
2	GAI	B	2009	-	3,3,3	0.77	0	3,3,3	0.94	0
2	GAI	A	2005	-	3,3,3	0.97	0	3,3,3	0.81	0
2	GAI	H	2016	-	3,3,3	1.05	0	3,3,3	1.75	1 (33%)
2	GAI	D	2010	-	3,3,3	1.01	0	3,3,3	1.28	0
2	GAI	J	2013	-	3,3,3	1.37	0	3,3,3	0.91	0
2	GAI	B	2004	-	3,3,3	0.48	0	3,3,3	0.30	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2014	GAI	C-N1	-2.44	1.23	1.30
2	E	2015	GAI	C-N2	-2.04	1.30	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2014	GAI	N3-C-N2	2.82	122.77	116.18
2	H	2016	GAI	N3-C-N2	2.59	122.24	116.18
2	C	2006	GAI	N3-C-N2	2.24	121.42	116.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2008	GAI	1	0
2	I	2012	GAI	1	0
2	F	2011	GAI	1	0
2	C	2001	GAI	1	0
2	E	2007	GAI	1	0
2	C	2006	GAI	1	0
2	B	2009	GAI	1	0
2	J	2013	GAI	1	0
2	B	2004	GAI	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, 95th 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 ²)	Q<0.9
1	A	200/203 (98%)	-0.28	1 (0%) 87 86	9, 20, 32, 37	0
1	B	200/203 (98%)	-0.42	0 100 100	9, 17, 29, 35	0
1	C	200/203 (98%)	-0.24	1 (0%) 87 86	11, 21, 33, 46	0
1	D	200/203 (98%)	0.02	2 (1%) 79 78	14, 26, 41, 53	0
1	E	200/203 (98%)	-0.48	0 100 100	9, 16, 28, 41	0
1	F	200/203 (98%)	1.47	70 (35%) 1 0	23, 47, 61, 64	0
1	G	200/203 (98%)	1.32	54 (27%) 1 1	11, 43, 58, 63	0
1	H	200/203 (98%)	-0.55	0 100 100	7, 14, 26, 31	0
1	I	200/203 (98%)	-0.49	0 100 100	7, 16, 27, 33	0
1	J	200/203 (98%)	-0.34	1 (0%) 87 86	10, 19, 34, 47	0
All	All	2000/2030 (98%)	0.00	129 (6%) 25 22	7, 21, 52, 64	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	667	PRO	5.5
1	G	593	GLY	4.1
1	F	607	ALA	4.0
1	G	568	TYR	4.0
1	G	532	VAL	3.8

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 oligosaccharides 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, 95th 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(\AA^2)	Q<0.9
2	GAI	C	2001	4/4	0.65	0.17	29,31,32,33	0
2	GAI	B	2004	4/4	0.74	0.13	19,23,23,24	0
2	GAI	A	2005	4/4	0.88	0.10	22,23,23,23	0
2	GAI	F	2011	4/4	0.90	0.09	32,32,32,32	0
2	GAI	D	2010	4/4	0.93	0.08	30,31,32,32	0
2	GAI	H	2017	4/4	0.93	0.09	35,35,36,36	0
2	GAI	H	2016	4/4	0.94	0.06	23,24,24,25	0
2	GAI	B	2009	4/4	0.94	0.07	14,15,15,16	0
2	GAI	C	2014	4/4	0.95	0.07	13,14,14,16	0
2	GAI	A	2002	4/4	0.95	0.06	14,16,17,17	0
2	GAI	E	2015	4/4	0.95	0.06	9,11,12,14	0
2	GAI	H	2008	4/4	0.97	0.05	14,14,15,16	0
2	GAI	C	2006	4/4	0.97	0.06	15,16,16,17	0
2	GAI	E	2007	4/4	0.97	0.04	10,10,10,11	0
2	GAI	I	2012	4/4	0.97	0.06	9,13,13,15	0
2	GAI	J	2013	4/4	0.97	0.05	10,10,10,12	0
2	GAI	B	2003	4/4	0.98	0.07	12,12,14,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.