



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:52 am GMT

PDB ID : 2PNL
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

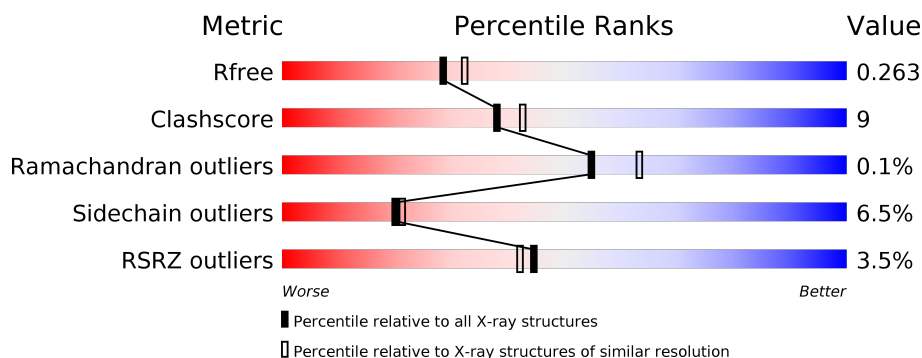
1 Overall quality at a glance

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.



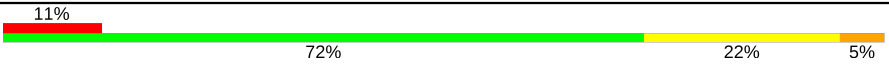



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4744 (2.24-2.20)
Clashscore	112137	5509 (2.24-2.20)
Ramachandran outliers	110173	5427 (2.24-2.20)
Sidechain outliers	110143	5428 (2.24-2.20)
RSRZ outliers	101464	4776 (2.24-2.20)

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 ≥ 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	203	<div> <div>85%</div> <div>15%</div> </div>
1	B	203	<div> <div>86%</div> <div>14%</div> </div>
1	C	203	<div> <div>85%</div> <div>12%</div> <div>•</div> </div>
1	D	203	<div> <div>78%</div> <div>18%</div> <div>•</div> </div>
1	E	203	<div> <div>83%</div> <div>15%</div> <div>•</div> </div>
1	F	203	<div> <div>22%</div> <div>62%</div> <div>33%</div> <div>5%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	203	
1	H	203	
1	I	203	
1	J	203	

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAI	B	2003	-	-	-	X
2	GAI	B	2004	-	-	-	X
2	GAI	C	2001	-	-	-	X
2	GAI	C	2006	-	X	-	-
2	GAI	C	2014	-	X	-	-
2	GAI	E	2007	-	-	-	X
2	GAI	H	2017	-	-	-	X

2 Entry composition

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

There are 40 discrepancies between the modelled and reference sequences:

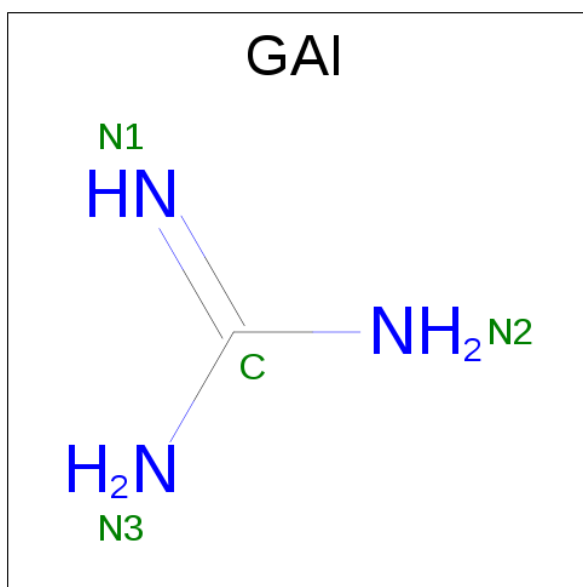
Chain	Residue	Modelled	Actual	Comment	Reference
A	603	MSE	MET	MODIFIED RESIDUE	UNP Q703G9
A	630	MSE	MET	MODIFIED RESIDUE	UNP Q703G9
A	652	MSE	MET	MODIFIED RESIDUE	UNP Q703G9
A	674	ALA	LYS	ENGINEERED	UNP Q703G9
B	603	MSE	MET	MODIFIED RESIDUE	UNP Q703G9
B	630	MSE	MET	MODIFIED RESIDUE	UNP Q703G9
B	652	MSE	MET	MODIFIED RESIDUE	UNP Q703G9
B	674	ALA	LYS	ENGINEERED	UNP Q703G9
C	603	MSE	MET	MODIFIED RESIDUE	UNP Q703G9

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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	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	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	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	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	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	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	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	UNP Q703G9

- Molecule 2 is GUANIDINE (three-letter code: 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		

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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.

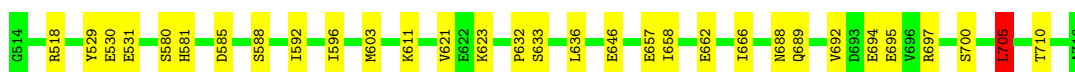
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	161	Total	O	0	0
			161	161		
3	C	141	Total	O	0	0
			141	141		
3	D	98	Total	O	0	0
			98	98		
3	E	145	Total	O	0	0
			145	145		
3	F	63	Total	O	0	0
			63	63		
3	G	66	Total	O	0	0
			66	66		
3	H	160	Total	O	0	0
			160	160		
3	I	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 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 VP4

Chain A: 




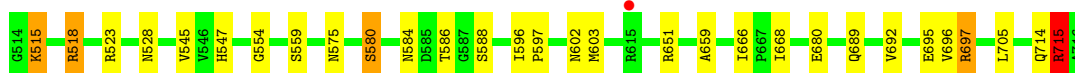
- Molecule 1: Protease VP4

Chain B: 




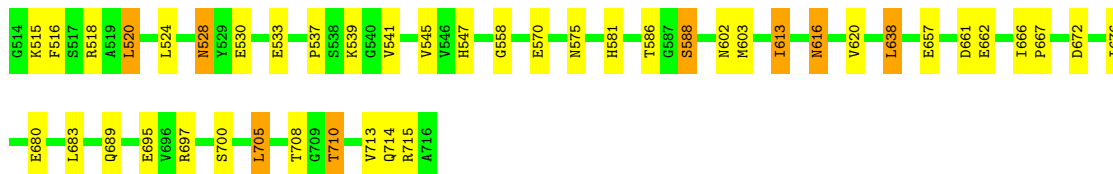
- Molecule 1: Protease VP4

Chain C: 




- Molecule 1: Protease VP4

Chain D: 



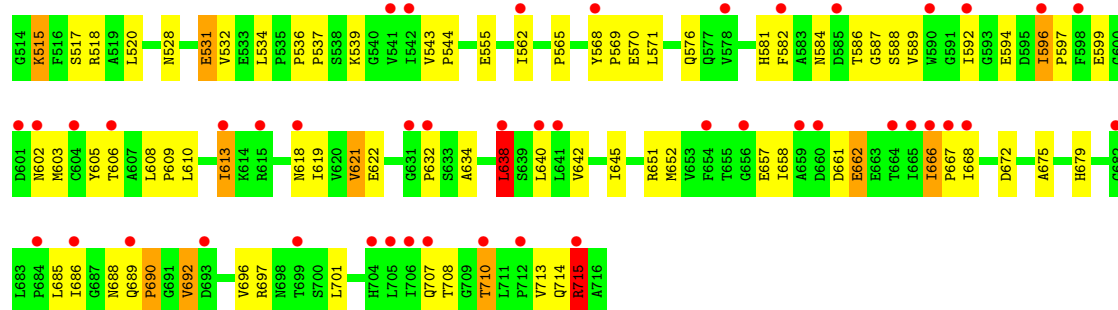
- Molecule 1: Protease VP4

Chain E: 

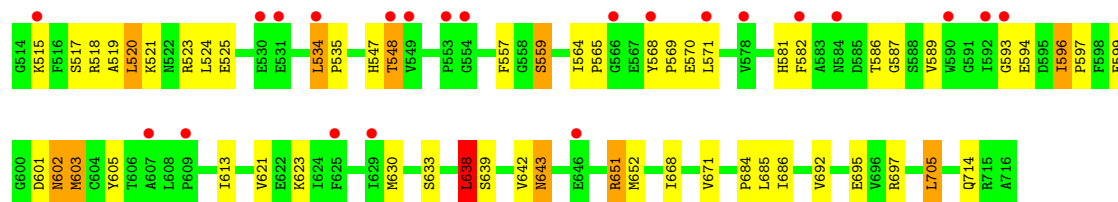




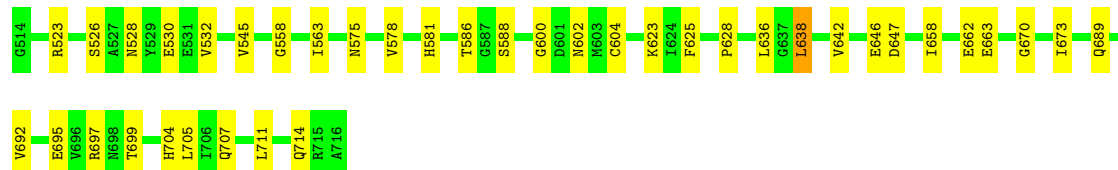
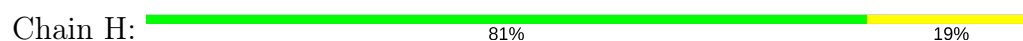
● Molecule 1: Protease VP4



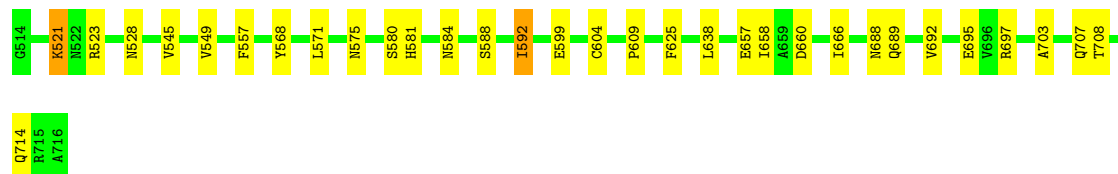
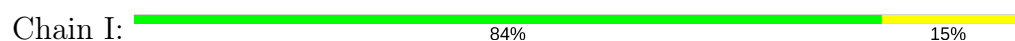
● Molecule 1: Protease VP4



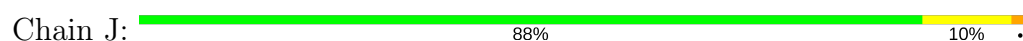
● Molecule 1: Protease VP4



● Molecule 1: Protease VP4



● Molecule 1: Protease VP4





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 48.14 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.3 (182.57-2.21) 96.2 (48.14-2.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.20Å)	Xtriage
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 (5.25%)	DCC
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16426	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

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	0.87	0/1536	0.81	1/2092 (0.0%)
1	B	0.89	0/1542	0.82	2/2099 (0.1%)
1	C	0.85	0/1542	0.84	2/2099 (0.1%)
1	D	0.80	0/1542	0.79	2/2099 (0.1%)
1	E	0.90	1/1546 (0.1%)	0.88	3/2103 (0.1%)
1	F	0.68	0/1540	0.72	1/2096 (0.0%)
1	G	0.74	0/1542	0.80	1/2099 (0.0%)
1	H	1.00	2/1543 (0.1%)	0.84	0/2099
1	I	0.95	1/1543 (0.1%)	0.84	0/2099
1	J	0.89	0/1536	0.85	3/2092 (0.1%)
All	All	0.86	4/15412 (0.0%)	0.82	15/20977 (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	1
1	F	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	604	CYS	CB-SG	8.66	1.97	1.82
1	I	604	CYS	CB-SG	5.50	1.91	1.82
1	H	526	SER	CB-OG	-5.07	1.35	1.42
1	E	669	CYS	CB-SG	5.02	1.90	1.82

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	651	ARG	NE-CZ-NH1	-10.34	115.13	120.30
1	J	651	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	E	584	ASN	C-N-CA	-7.13	103.88	121.70
1	G	638	LEU	CA-CB-CG	6.98	131.35	115.30
1	D	638	LEU	CA-CB-CG	5.89	128.86	115.30
1	B	518	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	651	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	E	520	LEU	CA-CB-CG	5.63	128.24	115.30
1	C	715	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	518	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	584	ASN	C-N-CA	-5.22	108.65	121.70
1	F	638	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	705	LEU	CB-CG-CD2	5.08	119.64	111.00
1	D	705	LEU	CA-CB-CG	5.03	126.87	115.30
1	J	711	LEU	CA-CB-CG	5.03	126.87	115.30

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 ⓘ

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	19	1
1	B	1515	0	1504	25	0
1	C	1515	0	1504	23	0
1	D	1515	0	1504	30	0
1	E	1519	0	1515	22	1
1	F	1513	0	1505	68	0
1	G	1515	0	1504	44	0
1	H	1516	0	1504	23	0
1	I	1516	0	1505	24	0
1	J	1509	0	1494	21	0
2	A	8	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	A	118	0	0	3	0
3	B	161	0	0	3	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	263	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.

All (263) 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
1:E:615:ARG:HH11	1:E:615:ARG:HG3	1.25	1.01
1:G:593:GLY:HA3	1:G:630:MSE:SE	2.10	1.01
1:J:582:PHE:CD2	1:J:596:ILE:CD1	2.53	0.92
1:J:676:ILE:O	1:J:680:GLU:HG3	1.69	0.92
1:D:695:GLU:H	1:E:575:ASN:HD21	1.20	0.90
1:F:582:PHE:CD2	1:F:596:ILE:CD1	2.55	0.88
1:B:695:GLU:H	1:C:575:ASN:HD21	1.24	0.85
1:F:589:VAL:HG13	1:F:605:TYR:HB2	1.60	0.84
1:F:658:ILE:CG2	1:F:662:GLU:HA	2.08	0.83
1:C:695:GLU:H	1:D:575:ASN:HD21	1.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:GLU:HG2	3:B:2073:HOH:O	1.78	0.81
1:G:586:THR:HG21	1:G:599:GLU:OE2	1.82	0.80
1:F:713:VAL:HB	1:G:548:THR:HG23	1.62	0.79
1:A:592:ILE:HD11	1:A:596:ILE:HD11	1.65	0.78
1:D:616:ASN:HD22	1:D:616:ASN:N	1.80	0.78
1:G:534:LEU:HD12	1:G:621:VAL:HG21	1.65	0.78
1:A:695:GLU:H	1:B:575:ASN:HD21	1.28	0.78
1:A:710:THR:HG22	3:A:2071:HOH:O	1.84	0.77
1:G:639:SER:O	1:G:643:ASN:HB2	1.84	0.77
1:J:582:PHE:HD2	1:J:596:ILE:CD1	1.97	0.77
1:I:584:ASN:ND2	1:I:599:GLU:OE2	2.17	0.76
1:E:662:GLU:HG3	3:E:2099:HOH:O	1.86	0.76
1:I:703:ALA:O	1:I:707:GLN:HG2	1.85	0.75
1:C:515:LYS:HD3	1:C:554:GLY:O	1.86	0.75
1:D:616:ASN:ND2	1:D:616:ASN:N	2.34	0.74
1:F:532:VAL:HG12	1:F:621:VAL:HG12	1.68	0.74
1:D:613:ILE:HD11	1:D:683:LEU:HD11	1.70	0.73
1:F:582:PHE:CG	1:F:596:ILE:HD11	2.23	0.73
1:F:714:GLN:HE21	1:G:547:HIS:HE1	1.36	0.73
1:F:565:PRO:HB3	1:F:603:MSE:HE2	1.71	0.73
1:F:688:ASN:HB2	1:F:696:VAL:O	1.89	0.72
1:F:582:PHE:CE2	1:F:596:ILE:HD11	2.26	0.70
1:C:697:ARG:NH1	1:D:530:GLU:OE1	2.25	0.70
1:D:710:THR:HG23	3:D:2024:HOH:O	1.92	0.70
1:D:616:ASN:H	1:D:616:ASN:ND2	1.90	0.69
1:C:689:GLN:O	1:C:692:VAL:HG22	1.93	0.69
1:F:613:ILE:N	1:F:613:ILE:HD12	2.08	0.69
1:I:581:HIS:HD2	1:I:588:SER:OG	1.75	0.68
1:F:515:LYS:HE2	3:F:2048:HOH:O	1.92	0.68
1:G:582:PHE:CD2	1:G:596:ILE:HD11	2.29	0.68
1:F:576:GLN:NE2	3:F:2074:HOH:O	2.26	0.67
1:B:695:GLU:H	1:C:575:ASN:ND2	1.93	0.67
1:B:565:PRO:HB3	1:B:603:MSE:HE1	1.77	0.66
1:F:613:ILE:H	1:F:613:ILE:HD12	1.60	0.66
1:E:613:ILE:HG23	1:E:619:ILE:HG22	1.77	0.66
1:G:547:HIS:NE2	1:G:559:SER:HB3	2.10	0.66
1:B:528:ASN:HD21	2:B:2009:GAI:HN21	1.44	0.66
1:D:520:LEU:HD22	1:D:524:LEU:HG	1.78	0.65
1:F:632:PRO:HB2	1:F:657:GLU:HB2	1.78	0.65
1:F:714:GLN:HE21	1:G:547:HIS:CE1	2.15	0.65
1:H:523:ARG:HD2	3:H:2064:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:531:GLU:HB2	1:F:622:GLU:HB3	1.77	0.65
1:H:695:GLU:H	1:I:575:ASN:HD21	1.44	0.64
1:A:688:ASN:HD21	1:A:697:ARG:HE	1.43	0.64
1:F:689:GLN:HB2	1:F:690:PRO:HD2	1.79	0.64
1:A:710:THR:HG23	3:A:2049:HOH:O	1.97	0.64
1:I:695:GLU:H	1:J:575:ASN:HD21	1.44	0.64
1:F:534:LEU:HD12	1:F:619:ILE:HD11	1.78	0.64
1:D:710:THR:CG2	3:D:2024:HOH:O	2.46	0.63
1:H:581:HIS:HD2	1:H:588:SER:OG	1.80	0.63
1:G:695:GLU:H	1:H:575:ASN:HD21	1.46	0.63
1:I:714:GLN:HE21	1:J:545:VAL:HG11	1.63	0.63
1:B:714:GLN:HE21	1:C:545:VAL:HG11	1.63	0.63
1:F:658:ILE:HG21	1:F:662:GLU:HG2	1.80	0.63
1:C:518:ARG:NH2	1:C:680:GLU:OE2	2.31	0.62
1:F:543:VAL:HG11	1:F:634:ALA:HA	1.83	0.61
1:G:685:LEU:HG	1:G:692:VAL:HG22	1.81	0.61
1:E:615:ARG:HG3	1:E:615:ARG:NH1	2.03	0.61
1:G:521:LYS:O	1:G:525:GLU:HG3	2.01	0.61
1:F:534:LEU:HB2	1:F:619:ILE:HG13	1.83	0.60
1:E:615:ARG:HH11	1:E:615:ARG:CG	2.08	0.60
1:C:528:ASN:HD21	2:C:2006:GAI:HN22	1.47	0.60
1:B:676:ILE:O	1:B:680:GLU:HG3	2.02	0.60
1:B:695:GLU:N	1:C:575:ASN:HD21	1.99	0.60
1:B:714:GLN:NE2	1:C:545:VAL:HG11	2.16	0.60
1:A:632:PRO:HB2	1:A:657:GLU:HG3	1.84	0.59
1:E:528:ASN:HD21	2:E:2007:GAI:HN22	1.48	0.59
1:E:565:PRO:HB3	1:E:603:MSE:CE	2.32	0.59
1:F:658:ILE:HG23	1:F:662:GLU:HA	1.84	0.59
1:G:582:PHE:HA	1:G:596:ILE:HG13	1.84	0.59
1:G:534:LEU:CD1	1:G:621:VAL:HG21	2.31	0.59
1:F:568:TYR:HB3	1:F:571:LEU:HD12	1.84	0.59
1:J:528:ASN:HD21	2:J:2013:GAI:HN22	1.51	0.59
1:A:710:THR:CG2	3:A:2049:HOH:O	2.50	0.59
1:J:633:SER:CB	1:J:668:ILE:HG21	2.27	0.59
1:F:666:ILE:HB	1:F:667:PRO:HD2	1.85	0.58
1:G:651:ARG:CG	1:G:651:ARG:HH21	2.17	0.58
1:F:589:VAL:HG13	1:F:605:TYR:CB	2.32	0.57
1:E:565:PRO:HB3	1:E:603:MSE:HE1	1.87	0.57
1:H:528:ASN:HD21	2:H:2008:GAI:HN32	1.51	0.56
1:J:581:HIS:HD2	1:J:588:SER:OG	1.88	0.56
1:F:569:PRO:HD2	1:F:570:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:PRO:HB3	1:B:603:MSE:CE	2.35	0.56
1:A:518:ARG:HB3	1:A:518:ARG:CZ	2.35	0.55
1:F:543:VAL:CG1	1:F:544:PRO:HD2	2.37	0.55
1:J:689:GLN:O	1:J:692:VAL:HG22	2.05	0.55
1:I:521:LYS:HB2	1:I:557:PHE:CG	2.42	0.55
1:E:581:HIS:HD2	1:E:588:SER:OG	1.88	0.55
1:F:652:MSE:HB2	1:F:686:ILE:CG1	2.37	0.55
1:I:657:GLU:HB3	1:I:666:ILE:HB	1.88	0.55
1:A:689:GLN:O	1:A:692:VAL:HG22	2.07	0.55
1:G:565:PRO:HB3	1:G:603:MSE:SE	2.56	0.55
1:F:581:HIS:HD2	1:F:588:SER:OG	1.90	0.55
1:F:657:GLU:HB3	1:F:666:ILE:HG13	1.88	0.54
1:B:703:ALA:O	1:B:707:GLN:HG3	2.06	0.54
1:G:638:LEU:O	1:G:642:VAL:HG22	2.07	0.54
1:C:696:VAL:HG23	1:C:696:VAL:O	2.08	0.53
1:G:582:PHE:CD2	1:G:596:ILE:CG1	2.92	0.53
1:A:657:GLU:HB3	1:A:666:ILE:HB	1.89	0.53
1:F:536:PRO:HD3	1:F:618:ASN:OD1	2.08	0.53
1:H:704:HIS:HD2	1:I:625:PHE:CD2	2.27	0.53
1:J:582:PHE:CE2	1:J:596:ILE:HD12	2.38	0.53
1:F:608:LEU:HB3	1:F:621:VAL:CG2	2.38	0.53
1:H:578:VAL:HG21	1:H:628:PRO:HG3	1.91	0.53
1:B:567:GLU:HG2	1:B:590:TRP:HE1	1.74	0.52
1:D:695:GLU:H	1:E:575:ASN:ND2	2.00	0.52
1:G:568:TYR:N	1:G:569:PRO:HD3	2.24	0.52
1:G:602:ASN:HD22	1:G:602:ASN:N	2.08	0.52
1:G:524:LEU:HD12	1:G:557:PHE:HE2	1.75	0.52
1:D:676:ILE:O	1:D:680:GLU:HG3	2.10	0.52
1:G:582:PHE:HD2	1:G:596:ILE:HD11	1.71	0.52
1:F:582:PHE:CE2	1:F:596:ILE:CD1	2.89	0.51
1:H:530:GLU:OE1	1:H:623:LYS:CE	2.59	0.51
1:H:586:THR:HA	1:H:602:ASN:HD22	1.75	0.51
1:G:589:VAL:HG22	1:G:605:TYR:HB2	1.92	0.51
1:G:571:LEU:O	1:G:623:LYS:HG2	2.10	0.51
1:D:537:PRO:HB2	1:D:539:LYS:O	2.11	0.51
1:F:657:GLU:HG2	1:F:666:ILE:HD11	1.93	0.51
1:G:602:ASN:ND2	1:G:602:ASN:N	2.58	0.51
1:F:608:LEU:HB3	1:F:621:VAL:HG21	1.93	0.51
1:I:689:GLN:O	1:I:692:VAL:HG22	2.11	0.51
1:H:528:ASN:ND2	3:H:2068:HOH:O	2.38	0.51
1:F:609:PRO:HG2	1:F:622:GLU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:596:ILE:HD11	1:J:598:PHE:CD1	2.47	0.50
1:A:705:LEU:HG	1:B:625:PHE:HZ	1.76	0.50
1:D:581:HIS:CD2	1:D:588:SER:HB3	2.47	0.50
1:H:545:VAL:O	1:H:558:GLY:HA2	2.12	0.50
1:C:586:THR:HA	1:C:602:ASN:HD22	1.76	0.50
1:J:521:LYS:HG3	1:J:557:PHE:CD1	2.47	0.50
1:H:636:LEU:HA	1:H:658:ILE:HD11	1.93	0.50
1:F:562:ILE:HB	1:F:610:LEU:HD22	1.93	0.50
1:F:658:ILE:HG21	1:F:662:GLU:HA	1.91	0.49
1:F:685:LEU:O	1:F:692:VAL:HG22	2.12	0.49
1:F:715:ARG:HG2	3:F:2034:HOH:O	2.11	0.49
1:H:530:GLU:OE1	1:H:623:LYS:NZ	2.45	0.49
1:I:688:ASN:HD21	1:I:697:ARG:HE	1.60	0.49
1:G:534:LEU:HD23	1:G:535:PRO:HD2	1.94	0.49
1:H:714:GLN:HB3	1:I:545:VAL:HG11	1.95	0.49
1:F:668:ILE:H	1:F:689:GLN:HE22	1.61	0.49
1:B:580:SER:O	1:B:588:SER:HB2	2.13	0.49
1:F:543:VAL:HG13	1:F:544:PRO:HD2	1.95	0.49
1:F:596:ILE:O	1:F:596:ILE:HG12	2.13	0.48
1:F:713:VAL:HB	1:G:548:THR:CG2	2.38	0.48
1:A:658:ILE:CG2	1:A:662:GLU:HA	2.43	0.48
1:G:714:GLN:HE21	1:H:545:VAL:HG11	1.77	0.48
1:D:520:LEU:CD2	1:D:524:LEU:HG	2.42	0.48
1:H:563:ILE:HD13	1:H:638:LEU:HD13	1.96	0.48
1:F:675:ALA:HB1	1:F:679:HIS:CE1	2.49	0.48
1:D:586:THR:HA	1:D:602:ASN:HD22	1.79	0.48
1:F:638:LEU:O	1:F:642:VAL:HG22	2.13	0.48
1:F:714:GLN:HG2	1:G:547:HIS:CE1	2.48	0.47
1:G:518:ARG:HH21	1:G:521:LYS:NZ	2.12	0.47
1:A:592:ILE:CD1	1:A:596:ILE:HD11	2.39	0.47
1:B:567:GLU:HG2	1:B:590:TRP:NE1	2.29	0.47
1:F:596:ILE:HA	1:F:597:PRO:HD3	1.75	0.47
1:I:581:HIS:CD2	1:I:588:SER:OG	2.62	0.47
1:G:601:ASP:OD2	1:G:605:TYR:OH	2.32	0.47
1:I:714:GLN:NE2	1:J:545:VAL:HG11	2.29	0.47
1:F:517:SER:CB	1:F:555:GLU:HB3	2.44	0.47
1:F:652:MSE:HB2	1:F:686:ILE:HG13	1.96	0.47
1:G:596:ILE:HA	1:G:597:PRO:HD3	1.64	0.47
1:D:657:GLU:HB3	1:D:666:ILE:HB	1.97	0.46
1:A:580:SER:HB2	1:A:592:ILE:HG13	1.95	0.46
1:E:570:GLU:HG3	1:E:570:GLU:H	1.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:582:PHE:HD1	1:F:587:GLY:C	2.19	0.46
1:H:670:GLY:HA2	3:H:2026:HOH:O	2.15	0.46
1:D:515:LYS:O	1:D:516:PHE:C	2.53	0.46
1:G:705:LEU:HG	1:H:625:PHE:HZ	1.81	0.46
1:H:689:GLN:O	1:H:692:VAL:HG22	2.15	0.46
1:B:523:ARG:HD3	3:B:2162:HOH:O	2.16	0.46
1:F:708:THR:C	1:F:710:THR:H	2.19	0.46
1:F:657:GLU:O	1:F:666:ILE:HG12	2.16	0.46
1:E:589:VAL:HG11	1:E:592:ILE:HD12	1.98	0.45
1:D:533:GLU:HG3	1:D:620:VAL:HG22	1.98	0.45
1:C:580:SER:O	1:C:588:SER:HB2	2.16	0.45
1:H:530:GLU:OE1	1:H:623:LYS:HE3	2.16	0.45
1:D:518:ARG:NH2	1:D:680:GLU:OE2	2.50	0.45
1:G:651:ARG:HH21	1:G:651:ARG:HG3	1.81	0.45
1:F:609:PRO:O	1:F:621:VAL:HG22	2.17	0.45
1:E:657:GLU:HB3	1:E:666:ILE:HB	1.98	0.45
1:G:582:PHE:CD2	1:G:596:ILE:CD1	2.99	0.45
1:F:543:VAL:CG1	1:F:544:PRO:CD	2.96	0.44
1:I:688:ASN:HD21	1:I:697:ARG:NE	2.15	0.44
1:G:519:ALA:O	1:G:523:ARG:HG3	2.18	0.44
1:F:714:GLN:NE2	1:G:547:HIS:HE1	2.08	0.44
1:C:559:SER:HB2	2:C:2001:GAI:N1	2.33	0.44
1:C:596:ILE:HA	1:C:597:PRO:HD3	1.86	0.44
1:D:714:GLN:NE2	1:E:545:VAL:HG11	2.33	0.44
1:G:517:SER:OG	1:G:520:LEU:HB2	2.18	0.44
1:I:592:ILE:CD1	3:I:2065:HOH:O	2.66	0.44
1:E:545:VAL:O	1:E:558:GLY:HA2	2.18	0.43
1:F:609:PRO:O	1:F:621:VAL:CG2	2.66	0.43
1:F:568:TYR:HB2	1:F:606:THR:HG21	2.00	0.43
1:G:652:MSE:HB2	1:G:686:ILE:HG12	2.00	0.43
1:D:545:VAL:O	1:D:558:GLY:HA2	2.17	0.43
1:G:582:PHE:HD1	1:G:587:GLY:C	2.22	0.43
1:I:568:TYR:HB3	1:I:571:LEU:HD12	2.00	0.43
1:F:640:LEU:O	1:F:645:ILE:HD12	2.18	0.43
1:B:688:ASN:ND2	3:B:2058:HOH:O	2.52	0.43
1:H:695:GLU:H	1:I:575:ASN:ND2	2.15	0.43
1:C:714:GLN:HG2	1:D:547:HIS:CE1	2.54	0.42
1:F:536:PRO:HA	1:F:537:PRO:HD3	1.79	0.42
1:A:530:GLU:OE1	1:A:623:LYS:HE3	2.19	0.42
1:D:667:PRO:HB3	1:D:689:GLN:HB3	2.02	0.42
1:E:516:PHE:HB2	1:E:673:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:580:SER:HB2	1:I:592:ILE:HG13	2.01	0.42
1:B:715:ARG:NH2	3:C:2111:HOH:O	2.52	0.42
1:F:586:THR:HA	1:F:602:ASN:ND2	2.34	0.42
1:D:714:GLN:HE21	1:E:547:HIS:HE1	1.66	0.42
1:I:695:GLU:H	1:J:575:ASN:ND2	2.13	0.42
1:G:633:SER:HB3	1:G:668:ILE:HG21	2.01	0.42
1:D:708:THR:HB	1:E:549:VAL:HG21	2.00	0.42
1:E:659:ALA:HB3	1:E:664:THR:HB	2.01	0.42
1:I:528:ASN:HD21	2:I:2012:GAI:HN32	1.67	0.42
1:I:523:ARG:NH2	3:I:2121:HOH:O	2.52	0.42
1:I:609:PRO:HD2	3:I:2099:HOH:O	2.20	0.42
1:C:692:VAL:CG2	1:C:695:GLU:HG2	2.50	0.42
1:F:610:LEU:HD21	1:F:613:ILE:HD11	2.02	0.41
1:D:714:GLN:HE21	1:E:545:VAL:HG11	1.85	0.41
1:I:708:THR:HB	1:J:549:VAL:HG21	2.02	0.41
1:B:636:LEU:HA	1:B:658:ILE:HD11	2.02	0.41
1:F:543:VAL:HG12	1:F:544:PRO:HD2	2.02	0.41
1:J:528:ASN:HD22	1:J:528:ASN:N	2.18	0.41
1:F:661:ASP:N	3:F:2059:HOH:O	2.53	0.41
1:G:652:MSE:HA	1:G:684:PRO:HD2	2.03	0.41
1:J:596:ILE:HG12	1:J:597:PRO:HD2	2.03	0.41
1:B:518:ARG:NH2	1:B:680:GLU:OE2	2.45	0.41
1:H:600:GLY:HA2	1:H:642:VAL:HG21	2.03	0.41
1:J:651:ARG:NH1	3:J:2082:HOH:O	2.48	0.41
1:B:697:ARG:HB3	1:B:701:LEU:HD12	2.02	0.41
1:C:523:ARG:NH2	3:C:2033:HOH:O	2.54	0.40
1:B:714:GLN:HE21	1:C:547:HIS:CE1	2.39	0.40
1:E:579:LEU:HD13	1:E:590:TRP:CE2	2.56	0.40
1:H:663:GLU:O	1:H:699:THR:HG23	2.22	0.40
1:A:531:GLU:OE1	1:A:611:LYS:NZ	2.39	0.40
1:A:529:TYR:CE1	1:A:623:LYS:HD2	2.56	0.40
1:A:636:LEU:HA	1:A:658:ILE:HD11	2.04	0.40
1:D:661:ASP:O	1:D:662:GLU:HB2	2.20	0.40
1:G:621:VAL:HG12	3:G:755:HOH:O	2.21	0.40
1:J:596:ILE:C	1:J:596:ILE:HD13	2.42	0.40
1:A:581:HIS:ND1	1:A:588:SER:OG	2.35	0.40
1:B:714:GLN:HB3	1:C:545:VAL:CG1	2.52	0.40
1:C:659:ALA:HB2	1:C:666:ILE:HD11	2.03	0.40
1:F:528:ASN:HD21	2:F:2011:GAI:HN31	1.68	0.40
1:B:559:SER:HB2	2:B:2004:GAI:N1	2.37	0.40
1:D:528:ASN:HD22	1:D:528:ASN:N	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:697:ARG:H	1:F:701:LEU:HD12	1.87	0.40
1:G:601:ASP:OD1	1:G:605:TYR:OH	2.38	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)
1:A:633:SER:OG	1:E:716:ALA:C[1_656]	1.99	0.21

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	201/203 (99%)	190 (94%)	11 (6%)	0	100	100
1	B	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	32	34
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%)	18	15
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%)	55	63

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 ⓘ

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%)	39	47
1	B	164/162 (101%)	160 (98%)	4 (2%)	54	66
1	C	164/162 (101%)	155 (94%)	9 (6%)	25	28
1	D	164/162 (101%)	149 (91%)	15 (9%)	11	10
1	E	165/162 (102%)	155 (94%)	10 (6%)	22	24
1	F	164/162 (101%)	144 (88%)	20 (12%)	6	4
1	G	164/162 (101%)	145 (88%)	19 (12%)	6	5
1	H	164/162 (101%)	154 (94%)	10 (6%)	22	24
1	I	164/162 (101%)	158 (96%)	6 (4%)	39	47
1	J	163/162 (101%)	155 (95%)	8 (5%)	29	34
All	All	1639/1620 (101%)	1532 (94%)	107 (6%)	20	21

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	603	MSE
1	A	621	VAL
1	A	646	GLU
1	A	694	GLU
1	A	700	SER
1	A	705	LEU
1	B	518	ARG
1	B	570	GLU
1	B	578	VAL
1	B	700	SER
1	C	515	LYS

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Mol	Chain	Res	Type
1	C	518	ARG
1	C	580	SER
1	C	603	MSE
1	C	651	ARG
1	C	668	ILE
1	C	697	ARG
1	C	705	LEU
1	C	715	ARG
1	D	520	LEU
1	D	528	ASN
1	D	541	VAL
1	D	570	GLU
1	D	588	SER
1	D	613	ILE
1	D	616	ASN
1	D	638	LEU
1	D	672	ASP
1	D	697	ARG
1	D	700	SER
1	D	705	LEU
1	D	710	THR
1	D	713	VAL
1	D	715	ARG
1	E	518	ARG
1	E	520	LEU
1	E	523	ARG
1	E	570	GLU
1	E	613	ILE
1	E	615	ARG
1	E	638	LEU
1	E	646	GLU
1	E	651	ARG
1	E	692	VAL
1	F	515	LYS
1	F	518	ARG
1	F	520	LEU
1	F	531	GLU
1	F	539	LYS
1	F	592	ILE
1	F	594	GLU
1	F	596	ILE
1	F	599	GLU

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Mol	Chain	Res	Type
1	F	613	ILE
1	F	621	VAL
1	F	638	LEU
1	F	651	ARG
1	F	662	GLU
1	F	666	ILE
1	F	672	ASP
1	F	692	VAL
1	F	707	GLN
1	F	710	THR
1	F	715	ARG
1	G	515	LYS
1	G	520	LEU
1	G	534	LEU
1	G	548	THR
1	G	559	SER
1	G	564	ILE
1	G	570	GLU
1	G	581	HIS
1	G	594	GLU
1	G	596	ILE
1	G	602	ASN
1	G	603	MSE
1	G	613	ILE
1	G	638	LEU
1	G	643	ASN
1	G	651	ARG
1	G	671	VAL
1	G	697	ARG
1	G	705	LEU
1	H	532	VAL
1	H	638	LEU
1	H	646	GLU
1	H	647	ASP
1	H	662	GLU
1	H	673	ILE
1	H	697	ARG
1	H	705	LEU
1	H	707	GLN
1	H	711	LEU
1	I	521	LYS
1	I	549	VAL

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Mol	Chain	Res	Type
1	I	592	ILE
1	I	638	LEU
1	I	658	ILE
1	I	660	ASP
1	J	515	LYS
1	J	535	PRO
1	J	596	ILE
1	J	633	SER
1	J	671	VAL
1	J	705	LEU
1	J	711	LEU
1	J	713	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	522	ASN
1	A	528	ASN
1	A	602	ASN
1	A	688	ASN
1	A	707	GLN
1	B	528	ASN
1	B	575	ASN
1	B	581	HIS
1	B	602	ASN
1	B	688	ASN
1	B	714	GLN
1	C	528	ASN
1	C	575	ASN
1	C	602	ASN
1	C	688	ASN
1	C	707	GLN
1	D	528	ASN
1	D	575	ASN
1	D	576	GLN
1	D	581	HIS
1	D	602	ASN
1	D	616	ASN
1	D	704	HIS
1	D	714	GLN
1	E	528	ASN
1	E	575	ASN

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Mol	Chain	Res	Type
1	E	576	GLN
1	E	581	HIS
1	E	602	ASN
1	E	643	ASN
1	E	688	ASN
1	F	528	ASN
1	F	581	HIS
1	F	602	ASN
1	F	689	GLN
1	F	714	GLN
1	G	528	ASN
1	G	576	GLN
1	G	602	ASN
1	G	643	ASN
1	G	688	ASN
1	G	714	GLN
1	H	528	ASN
1	H	575	ASN
1	H	581	HIS
1	H	602	ASN
1	H	688	ASN
1	H	704	HIS
1	H	714	GLN
1	I	528	ASN
1	I	575	ASN
1	I	581	HIS
1	I	602	ASN
1	I	688	ASN
1	I	704	HIS
1	I	714	GLN
1	J	528	ASN
1	J	575	ASN
1	J	581	HIS
1	J	602	ASN

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 [i](#)

There are no carbohydrates 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	A	2002	-	3,3,3	1.64	0	3,3,3	1.12	0
2	GAI	A	2005	-	3,3,3	1.50	0	3,3,3	0.81	0
2	GAI	B	2003	-	3,3,3	1.37	0	3,3,3	0.96	0
2	GAI	B	2004	-	3,3,3	0.52	0	3,3,3	0.31	0
2	GAI	B	2009	-	3,3,3	1.12	0	3,3,3	0.94	0
2	GAI	C	2001	-	3,3,3	0.13	0	3,3,3	0.99	0
2	GAI	C	2006	-	3,3,3	2.17	2 (66%)	3,3,3	1.50	1 (33%)
2	GAI	C	2014	-	3,3,3	2.34	2 (66%)	3,3,3	1.95	1 (33%)
2	GAI	D	2010	-	3,3,3	1.56	0	3,3,3	1.27	0
2	GAI	E	2007	-	3,3,3	0.96	0	3,3,3	0.84	0
2	GAI	E	2015	-	3,3,3	2.39	2 (66%)	3,3,3	0.29	0
2	GAI	F	2011	-	3,3,3	1.38	0	3,3,3	1.18	0
2	GAI	H	2008	-	3,3,3	1.94	2 (66%)	3,3,3	1.11	0
2	GAI	H	2016	-	3,3,3	1.53	1 (33%)	3,3,3	1.73	1 (33%)
2	GAI	H	2017	-	3,3,3	1.46	0	3,3,3	0.91	0
2	GAI	I	2012	-	3,3,3	1.39	0	3,3,3	1.01	0
2	GAI	J	2013	-	3,3,3	2.10	1 (33%)	3,3,3	0.91	0

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	GAI	A	2002	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAI	A	2005	-	-	0/0/0/0	0/0/0/0
2	GAI	B	2003	-	-	0/0/0/0	0/0/0/0
2	GAI	B	2004	-	-	0/0/0/0	0/0/0/0
2	GAI	B	2009	-	-	0/0/0/0	0/0/0/0
2	GAI	C	2001	-	-	0/0/0/0	0/0/0/0
2	GAI	C	2006	-	-	0/0/0/0	0/0/0/0
2	GAI	C	2014	-	-	0/0/0/0	0/0/0/0
2	GAI	D	2010	-	-	0/0/0/0	0/0/0/0
2	GAI	E	2007	-	-	0/0/0/0	0/0/0/0
2	GAI	E	2015	-	-	0/0/0/0	0/0/0/0
2	GAI	F	2011	-	-	0/0/0/0	0/0/0/0
2	GAI	H	2008	-	-	0/0/0/0	0/0/0/0
2	GAI	H	2016	-	-	0/0/0/0	0/0/0/0
2	GAI	H	2017	-	-	0/0/0/0	0/0/0/0
2	GAI	I	2012	-	-	0/0/0/0	0/0/0/0
2	GAI	J	2013	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2014	GAI	C-N1	-3.31	1.23	1.30
2	E	2015	GAI	C-N2	-3.13	1.30	1.36
2	J	2013	GAI	C-N2	-2.78	1.31	1.36
2	C	2006	GAI	C-N3	-2.70	1.31	1.36
2	H	2016	GAI	C-N1	-2.37	1.25	1.30
2	H	2008	GAI	C-N1	-2.27	1.25	1.30
2	H	2008	GAI	C-N2	-2.19	1.32	1.36
2	C	2006	GAI	C-N1	-2.17	1.26	1.30
2	E	2015	GAI	C-N3	-2.13	1.32	1.36
2	C	2014	GAI	C-N3	-2.12	1.32	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2006	GAI	N3-C-N2	2.22	121.42	116.13
2	H	2016	GAI	N3-C-N2	2.56	122.24	116.13
2	C	2014	GAI	N3-C-N2	2.79	122.77	116.13

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	B	2004	GAI	1	0
2	B	2009	GAI	1	0
2	C	2001	GAI	1	0
2	C	2006	GAI	1	0
2	E	2007	GAI	1	0
2	F	2011	GAI	1	0
2	H	2008	GAI	1	0
2	I	2012	GAI	1	0
2	J	2013	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

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, 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%)	-0.39	0 100 100	9, 20, 32, 37	0
1	B	200/203 (98%)	-0.45	1 (0%) 90 90	9, 17, 29, 35	0
1	C	200/203 (98%)	-0.38	1 (0%) 90 90	11, 21, 33, 46	0
1	D	200/203 (98%)	-0.28	0 100 100	14, 26, 41, 53	0
1	E	200/203 (98%)	-0.46	0 100 100	9, 16, 28, 41	0
1	F	200/203 (98%)	1.08	45 (22%) 1 1	23, 47, 61, 64	0
1	G	200/203 (98%)	0.67	22 (11%) 6 5	11, 43, 58, 63	0
1	H	200/203 (98%)	-0.43	0 100 100	7, 14, 26, 31	0
1	I	200/203 (98%)	-0.47	0 100 100	7, 16, 27, 33	0
1	J	200/203 (98%)	-0.44	0 100 100	10, 19, 34, 47	0
All	All	2000/2030 (98%)	-0.16	69 (3%) 44 42	7, 21, 52, 64	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	667	PRO	6.2
1	F	568	TYR	5.4
1	F	659	ALA	4.5
1	F	582	PHE	4.2
1	F	660	ASP	4.0
1	G	553	PRO	4.0
1	F	668	ILE	3.8
1	F	682	GLY	3.8
1	F	592	ILE	3.5
1	G	568	TYR	3.5
1	G	593	GLY	3.5
1	G	578	VAL	3.4
1	F	640	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	615	ARG	3.1
1	G	584	ASN	3.1
1	G	629	ILE	3.1
1	F	541	VAL	3.1
1	C	615	ARG	2.9
1	F	590	TRP	2.9
1	F	706	ILE	2.9
1	G	592	ILE	2.9
1	G	554	GLY	2.8
1	F	699	THR	2.8
1	F	693	ASP	2.8
1	F	596	ILE	2.8
1	F	664	THR	2.7
1	F	562	ILE	2.7
1	F	542	ILE	2.7
1	F	604	CYS	2.6
1	F	666	ILE	2.6
1	G	590	TRP	2.6
1	F	638	LEU	2.6
1	G	646	GLU	2.6
1	F	606	THR	2.5
1	F	665	ILE	2.5
1	F	686	ILE	2.5
1	G	571	LEU	2.5
1	F	613	ILE	2.5
1	F	715	ARG	2.5
1	G	515	LYS	2.4
1	F	578	VAL	2.3
1	F	704	HIS	2.3
1	F	707	GLN	2.3
1	G	566	GLY	2.3
1	F	712	PRO	2.3
1	F	585	ASP	2.3
1	G	534	LEU	2.3
1	F	602	ASN	2.3
1	F	654	PHE	2.2
1	G	548	THR	2.2
1	F	601	ASP	2.2
1	G	549	VAL	2.2
1	F	618	ASN	2.2
1	F	641	LEU	2.2
1	F	632	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	684	PRO	2.1
1	F	598	PHE	2.1
1	F	689	GLN	2.1
1	B	716	ALA	2.1
1	G	530	GLU	2.1
1	F	705	LEU	2.1
1	G	531	GLU	2.1
1	F	710	THR	2.1
1	F	656	GLY	2.0
1	G	607	ALA	2.0
1	G	609	PRO	2.0
1	G	582	PHE	2.0
1	G	625	PHE	2.0
1	F	631	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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GAI	C	2001	4/4	0.70	0.22	6.32	29,31,32,33	0
2	GAI	B	2004	4/4	0.83	0.16	4.95	19,23,23,24	0
2	GAI	B	2003	4/4	0.99	0.14	4.00	12,12,14,15	0
2	GAI	E	2007	4/4	0.98	0.13	2.31	10,10,10,11	0
2	GAI	H	2017	4/4	0.96	0.20	2.12	35,35,36,36	0
2	GAI	C	2014	4/4	0.97	0.15	1.72	13,14,14,16	0
2	GAI	C	2006	4/4	0.98	0.12	1.16	15,16,16,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GAI	A	2002	4/4	0.97	0.13	1.11	14,16,17,17	0
2	GAI	E	2015	4/4	0.97	0.12	0.44	9,11,12,14	0
2	GAI	J	2013	4/4	0.98	0.11	0.32	10,10,10,12	0
2	GAI	F	2011	4/4	0.96	0.13	0.11	32,32,32,32	0
2	GAI	B	2009	4/4	0.96	0.10	-0.32	14,15,15,16	0
2	GAI	D	2010	4/4	0.96	0.10	-0.45	30,31,32,32	0
2	GAI	I	2012	4/4	0.97	0.10	-0.85	9,13,13,15	0
2	GAI	H	2008	4/4	0.99	0.09	-0.91	14,14,15,16	0
2	GAI	H	2016	4/4	0.95	0.10	-0.97	23,24,24,25	0
2	GAI	A	2005	4/4	0.92	0.14	-	22,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.