



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:06 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 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

<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

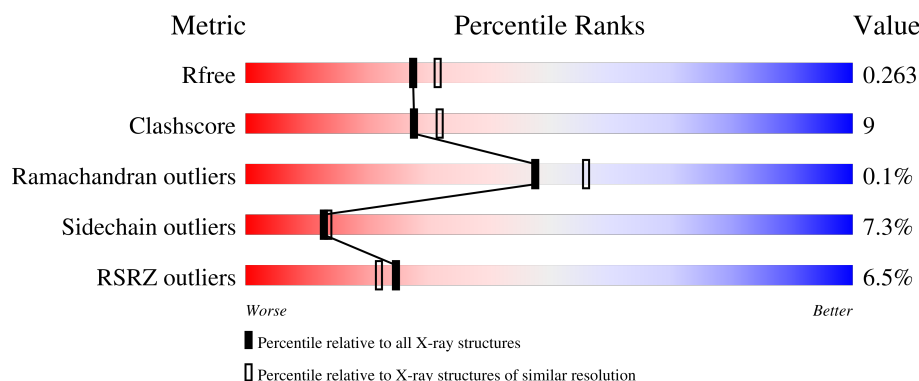
1 Overall quality at a glance

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.



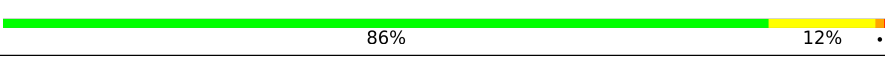
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	
1	B	203	
1	C	203	
1	D	203	
1	E	203	

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

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:

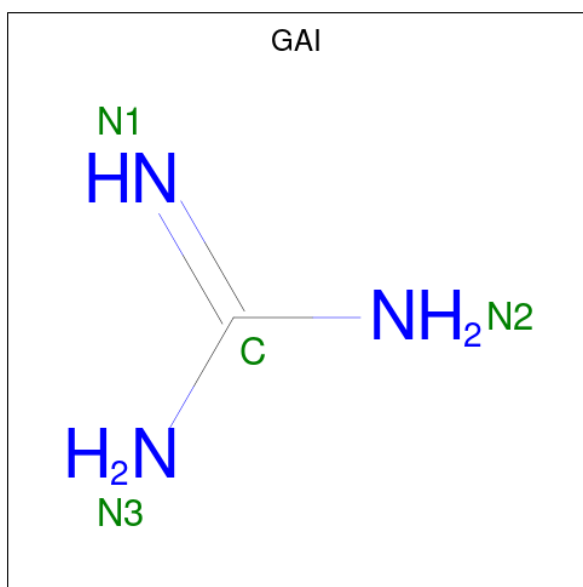
Chain	Residue	Modelled	Actual	Comment	Reference
A	603	MSE	MET	modified residue	UNP Q703G9
A	630	MSE	MET	modified residue	UNP Q703G9
A	652	MSE	MET	modified residue	UNP Q703G9
A	674	ALA	LYS	engineered mutation	UNP Q703G9
B	603	MSE	MET	modified residue	UNP Q703G9
B	630	MSE	MET	modified residue	UNP Q703G9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

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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 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: CH_5N_3).



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		

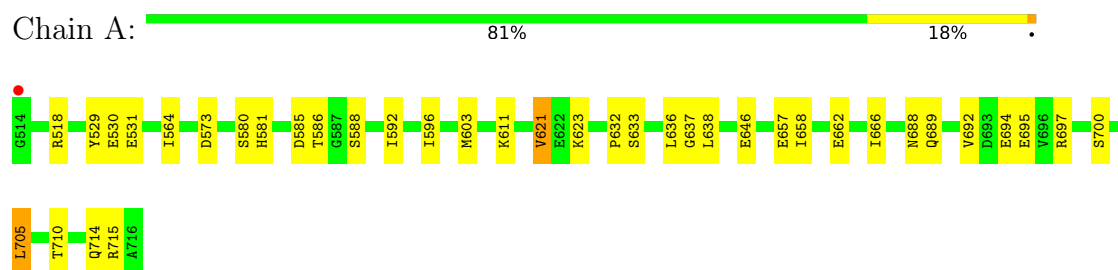
- Molecule 3 is water.

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		

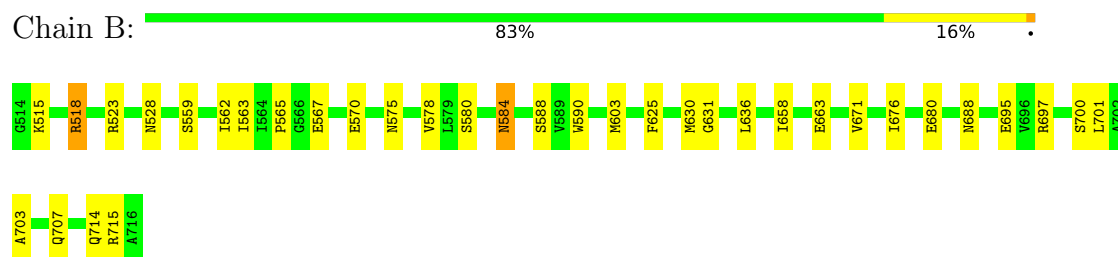
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

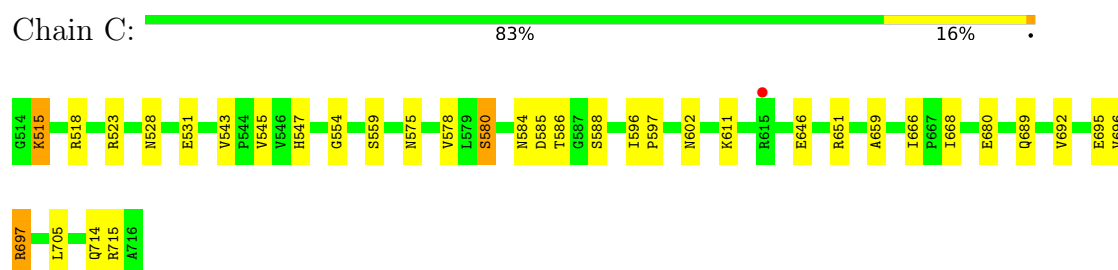
• Molecule 1: Protease VP4



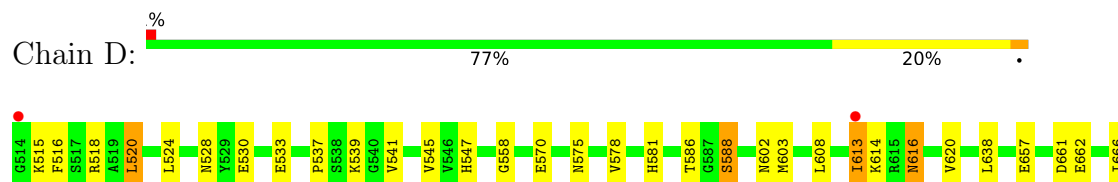
• Molecule 1: Protease VP4



• Molecule 1: Protease VP4



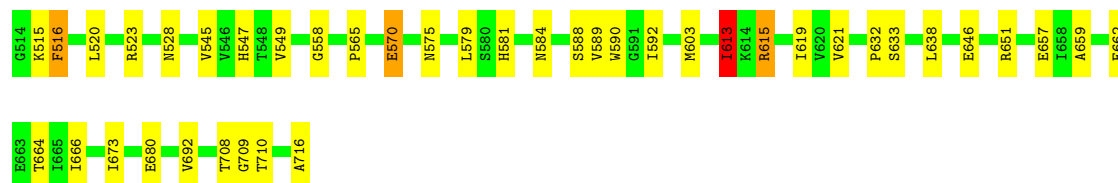
• Molecule 1: Protease VP4





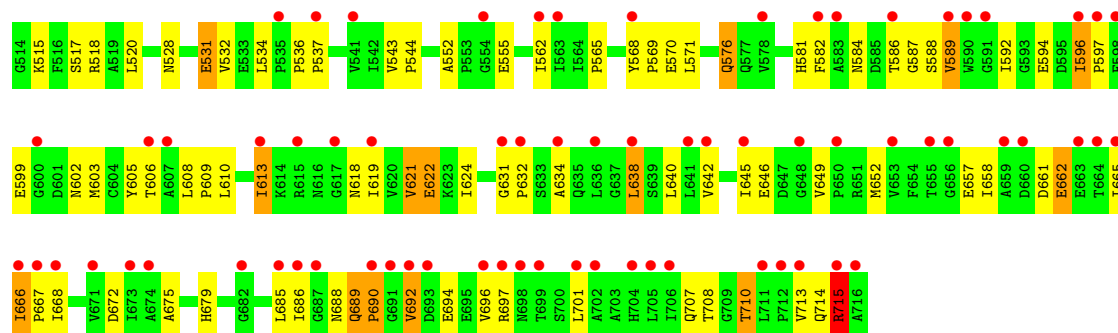
• Molecule 1: Protease VP4

Chain E: 80% 18%



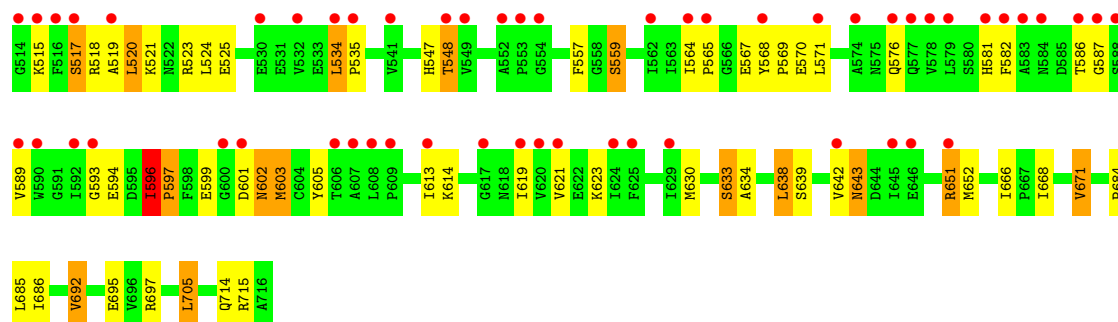
• Molecule 1: Protease VP4

Chain F: 34% 59% 33% 7%



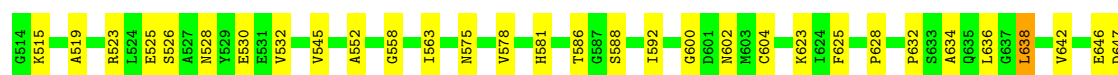
• Molecule 1: Protease VP4

Chain G: 27% 69% 23% 7%



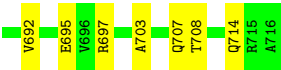
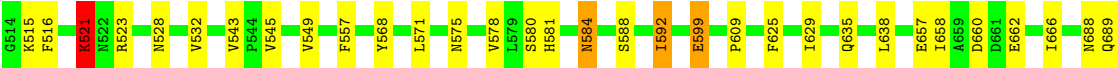
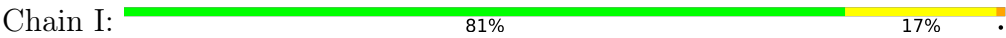
• Molecule 1: Protease VP4

Chain H: 77% 22%

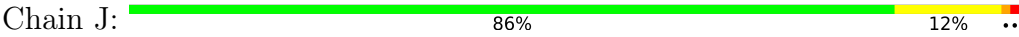




● Molecule 1: Protease VP4



● 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 – 2.21 182.57 – 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)	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 (4.91%)	wwPDB-VP
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 , 43.0	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	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

All (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
1	E	632	PRO	C-O	-6.45	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	630	MSE	SE-CE	-6.34	1.76	1.95
1	C	543	VAL	CA-CB	6.26	1.62	1.54
1	A	638	LEU	C-O	-6.17	1.16	1.24
1	A	714	GLN	C-O	-6.16	1.16	1.24
1	G	666	ILE	CA-CB	6.08	1.60	1.53
1	E	633	SER	C-O	-6.02	1.16	1.24
1	J	515	LYS	C-O	-5.96	1.16	1.23
1	H	634	ALA	CA-CB	-5.92	1.42	1.53
1	B	562	ILE	CA-CB	5.82	1.61	1.54
1	H	632	PRO	C-O	-5.80	1.16	1.24
1	F	649	VAL	CA-CB	5.80	1.59	1.54
1	B	630	MSE	C-O	-5.80	1.16	1.23
1	H	525	GLU	C-O	-5.79	1.16	1.24
1	A	637	GLY	C-O	-5.75	1.17	1.23
1	B	563	ILE	CA-CB	5.66	1.60	1.54
1	E	516	PHE	C-O	-5.61	1.17	1.23
1	H	666	ILE	CA-CB	5.54	1.59	1.53
1	B	631	GLY	C-O	-5.48	1.16	1.24
1	J	596	ILE	CA-C	5.47	1.57	1.52
1	G	715	ARG	C-O	-5.43	1.18	1.24
1	E	515	LYS	C-O	-5.32	1.17	1.23
1	A	715	ARG	C-O	-5.32	1.18	1.24
1	B	630	MSE	CG-SE	-5.21	1.79	1.95
1	H	515	LYS	C-O	-5.16	1.17	1.24
1	B	671	VAL	CA-CB	5.14	1.61	1.54
1	H	552	ALA	CA-CB	5.03	1.59	1.53
1	A	564	ILE	CA-C	5.01	1.56	1.52
1	H	634	ALA	C-O	-5.01	1.17	1.24

All (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
1	G	596	ILE	CA-C-N	9.68	129.30	119.82
1	G	596	ILE	C-N-CA	9.68	129.30	119.82
1	I	584	ASN	CA-C-N	-8.33	111.86	123.03
1	I	584	ASN	C-N-CA	-8.33	111.86	123.03
1	F	631	GLY	CA-C-N	7.62	127.79	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	631	GLY	C-N-CA	7.62	127.79	119.87
1	F	715	ARG	N-CA-C	7.13	121.01	107.75
1	G	619	ILE	N-CA-C	6.84	117.74	107.75
1	G	671	VAL	CB-CA-C	-6.78	102.98	112.14
1	B	584	ASN	CA-C-N	-6.47	114.36	123.03
1	B	584	ASN	C-N-CA	-6.47	114.36	123.03
1	J	651	ARG	NE-CZ-NH1	-6.37	115.13	121.50
1	G	634	ALA	N-CA-C	-6.36	104.78	113.30
1	J	671	VAL	CB-CA-C	-6.31	103.62	112.14
1	G	597	PRO	N-CA-C	6.20	121.98	113.98
1	J	595	ASP	CA-C-N	-6.08	117.44	123.04
1	J	595	ASP	C-N-CA	-6.08	117.44	123.04
1	F	552	ALA	CA-C-N	6.07	125.28	118.97
1	F	552	ALA	C-N-CA	6.07	125.28	118.97
1	J	596	ILE	N-CA-C	5.98	115.11	108.05
1	H	604	CYS	CB-CA-C	5.94	119.45	109.48
1	G	633	SER	N-CA-C	5.80	119.83	112.87
1	F	622	GLU	N-CA-C	5.70	117.46	108.96
1	E	709	GLY	N-CA-C	-5.70	106.64	114.67
1	G	517	SER	N-CA-C	5.58	117.49	108.34
1	J	651	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	E	613	ILE	CB-CA-C	-5.53	103.41	110.98
1	J	627	GLY	CA-C-N	5.51	125.49	120.03
1	J	627	GLY	C-N-CA	5.51	125.49	120.03
1	A	621	VAL	N-CA-CB	-5.32	103.53	112.47
1	I	521	LYS	N-CA-C	5.31	116.76	110.97
1	C	585	ASP	CB-CA-C	5.27	119.78	111.72
1	A	586	THR	N-CA-C	5.22	118.46	112.57
1	H	519	ALA	N-CA-C	5.04	116.77	111.28
1	I	635	GLN	N-CA-C	5.01	116.74	111.28
1	D	608	LEU	CA-C-N	-5.00	114.80	119.90
1	D	608	LEU	C-N-CA	-5.00	114.80	119.90

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	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
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.

All (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
1:E:615:ARG:HG3	1:E:615:ARG:HH11	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
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:N	1:D:616:ASN:HD22	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:N	1:D:616:ASN:ND2	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:ND2	1:D:616:ASN:H	1.90	0.69
1:C:689:GLN:O	1:C:692:VAL:HG22	1.93	0.69
1:F:613:ILE:HD12	1:F:613:ILE:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:F:613:ILE:H	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:658:ILE:HG23	1:F:662:GLU:HA	1.84	0.59
1:G:534:LEU:CD1	1:G:621:VAL:HG21	2.31	0.59
1:G:582:PHE:HA	1:G:596:ILE:HG13	1.84	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:HH21	1:G:651:ARG:CG	2.17	0.58
1:F:589:VAL:HG13	1:F:605:TYR:CB	2.32	0.57
1:G:601:ASP:CG	1:G:605:TYR:HH	2.13	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
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:O	1:C:696:VAL:HG23	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:N	1:G:602:ASN:HD22	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:571:LEU:O	1:G:623:LYS:HG2	2.10	0.51
1:G:589:VAL:HG22	1:G:605:TYR:HB2	1.92	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:N	1:G:602:ASN:ND2	2.58	0.51
1:F:608:LEU:HB3	1:F:621:VAL:HG21	1.93	0.51
1:F:708:THR:C	1:F:710:THR:H	2.19	0.51
1:I:689:GLN:O	1:I:692:VAL:HG22	2.11	0.51
1:D:515:LYS:O	1:D:516:PHE:C	2.53	0.51
1:F:582:PHE:HD1	1:F:587:GLY:C	2.19	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
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:B:515:LYS:NZ	3:B:2133:HOH:O	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:582:PHE:HD1	1:G:587:GLY:C	2.22	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:H	1:E:570:GLU:HG3	1.34	0.46
1:H:670:GLY:HA2	3:H:2026:HOH:O	2.15	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: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:C:531:GLU:OE1	1:C:611:LYS:NZ	2.39	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:J:596:ILE:HD13	1:J:596:ILE:C	2.42	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:A:529:TYR:OH	1:A:573:ASP:OD1	2.33	0.44
1:G:567:GLU:C	1:G:568:TYR:CD2	2.95	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:E:708:THR:C	1:E:710:THR:H	2.27	0.42
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:F:528:ASN:CG	1:F:624:ILE:HG22	2.45	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:523:ARG:NH2	3:I:2121:HOH:O	2.52	0.42
1:I:528:ASN:HD21	2:I:2012:GAI:HN32	1.67	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:I:515:LYS:O	1:I:516:PHE:C	2.62	0.41
1:J:528:ASN:N	1:J:528:ASN:HD22	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:714:GLN:HE21	1:C:547:HIS:CE1	2.39	0.40
1:C:523:ARG:NH2	3:C:2033:HOH:O	2.54	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:529:TYR:CE1	1:A:623:LYS:HD2	2.56	0.40
1:A:531:GLU:OE1	1:A:611:LYS:NZ	2.39	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:G:601:ASP:OD1	1:G:605:TYR:OH	2.38	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:G:596:ILE:HD12	1:G:596:ILE:C	2.45	0.40
1:B:559:SER:HB2	2:B:2004:GAI:N1	2.37	0.40
1:D:528:ASN:N	1:D:528:ASN:HD22	2.18	0.40
1:F:697:ARG:H	1:F:701:LEU:HD12	1.87	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%)	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 ⓘ

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	164/162 (101%)	142 (87%)	22 (13%)	4	3
1	H	164/162 (101%)	154 (94%)	10 (6%)	17	19
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

All (119) 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
1	C	578	VAL
1	C	580	SER
1	C	646	GLU
1	C	651	ARG
1	C	668	ILE
1	C	697	ARG
1	C	705	LEU
1	D	520	LEU
1	D	541	VAL
1	D	570	GLU
1	D	578	VAL
1	D	588	SER
1	D	613	ILE
1	D	614	LYS
1	D	616	ASN
1	D	638	LEU
1	D	672	ASP
1	D	700	SER
1	D	705	LEU
1	D	710	THR
1	D	713	VAL

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Mol	Chain	Res	Type
1	D	715	ARG
1	E	520	LEU
1	E	523	ARG
1	E	570	GLU
1	E	613	ILE
1	E	615	ARG
1	E	621	VAL
1	E	638	LEU
1	E	646	GLU
1	E	651	ARG
1	E	680	GLU
1	E	692	VAL
1	F	518	ARG
1	F	520	LEU
1	F	531	GLU
1	F	576	GLN
1	F	589	VAL
1	F	592	ILE
1	F	594	GLU
1	F	596	ILE
1	F	599	GLU
1	F	613	ILE
1	F	621	VAL
1	F	638	LEU
1	F	646	GLU
1	F	662	GLU
1	F	665	ILE
1	F	666	ILE
1	F	672	ASP
1	F	689	GLN
1	F	692	VAL
1	F	694	GLU
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

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Mol	Chain	Res	Type
1	G	576	GLN
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	614	LYS
1	G	638	LEU
1	G	643	ASN
1	G	651	ARG
1	G	671	VAL
1	G	692	VAL
1	G	697	ARG
1	G	705	LEU
1	H	532	VAL
1	H	592	ILE
1	H	638	LEU
1	H	646	GLU
1	H	647	ASP
1	H	662	GLU
1	H	673	ILE
1	H	705	LEU
1	H	707	GLN
1	H	711	LEU
1	I	521	LYS
1	I	532	VAL
1	I	549	VAL
1	I	578	VAL
1	I	592	ILE
1	I	638	LEU
1	I	658	ILE
1	I	660	ASP
1	I	662	GLU
1	J	515	LYS
1	J	518	ARG
1	J	578	VAL
1	J	596	ILE
1	J	633	SER
1	J	651	ARG
1	J	671	VAL
1	J	695	GLU

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Mol	Chain	Res	Type
1	J	705	LEU
1	J	711	LEU
1	J	713	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	522	ASN
1	A	528	ASN
1	A	602	ASN
1	A	643	ASN
1	A	688	ASN
1	A	707	GLN
1	B	528	ASN
1	B	575	ASN
1	B	581	HIS
1	B	643	ASN
1	B	681	GLN
1	B	688	ASN
1	B	707	GLN
1	B	714	GLN
1	C	528	ASN
1	C	575	ASN
1	C	602	ASN
1	C	643	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
1	E	581	HIS
1	E	602	ASN
1	E	688	ASN
1	F	528	ASN
1	F	581	HIS

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Mol	Chain	Res	Type
1	F	602	ASN
1	F	643	ASN
1	F	689	GLN
1	F	714	GLN
1	G	528	ASN
1	G	576	GLN
1	G	577	GLN
1	G	602	ASN
1	G	643	ASN
1	G	704	HIS
1	G	707	GLN
1	G	714	GLN
1	H	528	ASN
1	H	575	ASN
1	H	581	HIS
1	H	602	ASN
1	H	643	ASN
1	H	681	GLN
1	H	688	ASN
1	H	704	HIS
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
1	J	643	ASN
1	J	681	GLN

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 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($^{\circ}$)	Ideal($^{\circ}$)
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 ⓘ

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%)	-0.28	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

All (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
1	F	711	LEU	3.7
1	F	665	ILE	3.6
1	F	690	PRO	3.6
1	G	553	PRO	3.6
1	G	584	ASN	3.6
1	F	668	ILE	3.6
1	F	631	GLY	3.5
1	F	659	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	590	TRP	3.4
1	G	578	VAL	3.3
1	G	579	LEU	3.3
1	F	568	TYR	3.3
1	G	571	LEU	3.3
1	F	613	ILE	3.3
1	G	582	PHE	3.2
1	F	692	VAL	3.2
1	G	601	ASP	3.1
1	F	606	THR	3.1
1	G	564	ILE	3.0
1	F	582	PHE	3.0
1	G	554	GLY	3.0
1	F	632	PRO	3.0
1	F	666	ILE	3.0
1	F	686	ILE	3.0
1	G	517	SER	3.0
1	F	713	VAL	2.9
1	G	583	ALA	2.9
1	F	656	GLY	2.8
1	D	613	ILE	2.8
1	F	697	ARG	2.8
1	F	638	LEU	2.8
1	F	664	THR	2.8
1	G	592	ILE	2.8
1	G	629	ILE	2.8
1	G	565	PRO	2.8
1	F	541	VAL	2.8
1	G	621	VAL	2.8
1	G	642	VAL	2.8
1	F	696	VAL	2.8
1	G	552	ALA	2.7
1	F	578	VAL	2.7
1	F	671	VAL	2.7
1	G	645	ILE	2.7
1	G	600	GLY	2.7
1	F	648	GLY	2.7
1	G	586	THR	2.6
1	F	583	ALA	2.6
1	F	642	VAL	2.6
1	F	687	GLY	2.6
1	F	685	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	597	PRO	2.6
1	G	514	GLY	2.6
1	G	589	VAL	2.5
1	D	514	GLY	2.5
1	G	515	LYS	2.5
1	G	574	ALA	2.5
1	F	653	VAL	2.5
1	G	581	HIS	2.5
1	G	534	LEU	2.4
1	J	514	GLY	2.4
1	F	701	LEU	2.4
1	F	705	LEU	2.4
1	F	698	ASN	2.4
1	G	607	ALA	2.4
1	G	548	THR	2.4
1	G	516	PHE	2.4
1	G	613	ILE	2.4
1	G	646	GLU	2.4
1	G	549	VAL	2.4
1	F	699	THR	2.3
1	G	608	LEU	2.3
1	F	650	PRO	2.3
1	F	655	THR	2.3
1	G	624	ILE	2.3
1	F	712	PRO	2.3
1	A	514	GLY	2.3
1	G	577	GLN	2.3
1	G	587	GLY	2.3
1	G	519	ALA	2.3
1	G	609	PRO	2.2
1	F	600	GLY	2.2
1	F	682	GLY	2.2
1	F	715	ARG	2.2
1	G	617	GLY	2.2
1	F	562	ILE	2.2
1	F	636	LEU	2.2
1	C	615	ARG	2.2
1	G	535	PRO	2.2
1	G	651	ARG	2.2
1	F	535	PRO	2.2
1	F	716	ALA	2.2
1	G	620	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	704	HIS	2.2
1	G	576	GLN	2.2
1	G	588	SER	2.2
1	G	562	ILE	2.1
1	F	589	VAL	2.1
1	F	660	ASP	2.1
1	G	541	VAL	2.1
1	F	617	GLY	2.1
1	F	586	THR	2.1
1	G	530	GLU	2.1
1	F	598	PHE	2.1
1	G	606	THR	2.1
1	F	563	ILE	2.1
1	F	537	PRO	2.1
1	G	625	PHE	2.1
1	F	554	GLY	2.1
1	F	634	ALA	2.1
1	F	702	ALA	2.1
1	F	596	ILE	2.1
1	F	619	ILE	2.1
1	F	645	ILE	2.1
1	F	591	GLY	2.1
1	F	691	GLY	2.1
1	F	663	GLU	2.0
1	F	641	LEU	2.0
1	F	693	ASP	2.0
1	F	706	ILE	2.0
1	G	619	ILE	2.0
1	F	615	ARG	2.0
1	F	590	TRP	2.0
1	F	674	ALA	2.0
1	F	673	ILE	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 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($\text{\AA}^2$)	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.