



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:25 AM UTC

PDB ID : 4S1T / pdb_00004s1t
Title : Crystal structure of the mutant I26A/N52A of the endoribonuclease from human coronavirus 229E
Authors : Huo, T.; Liu, X.
Deposited on : 2015-01-15
Resolution : 2.50 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

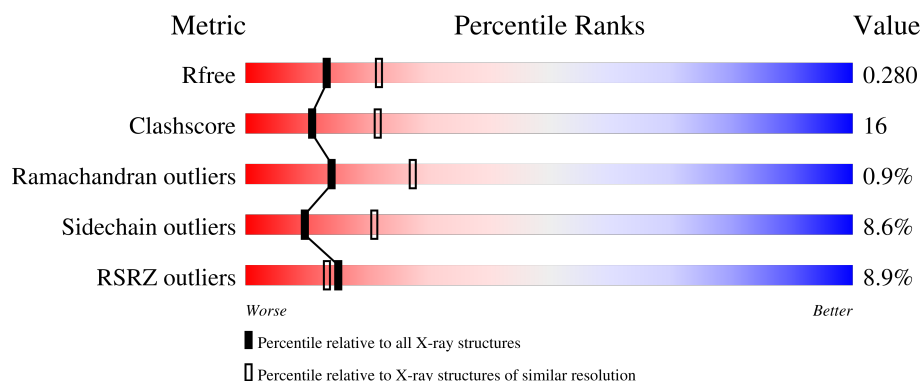
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	349	
1	B	349	
1	C	349	
1	D	349	
1	E	349	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	349	6% 71% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16623 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 Uridylate-specific endoribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2679	1728	433	505	13			
1	B	342	Total	C	N	O	S	0	0	0
			2679	1728	433	505	13			
1	C	342	Total	C	N	O	S	0	0	0
			2679	1728	433	505	13			
1	D	342	Total	C	N	O	S	0	0	0
			2679	1728	433	505	13			
1	E	342	Total	C	N	O	S	0	0	0
			2679	1728	433	505	13			
1	F	342	Total	C	N	O	S	0	0	0
			2679	1728	433	505	13			

There are 18 discrepancies between the modelled and reference sequences:

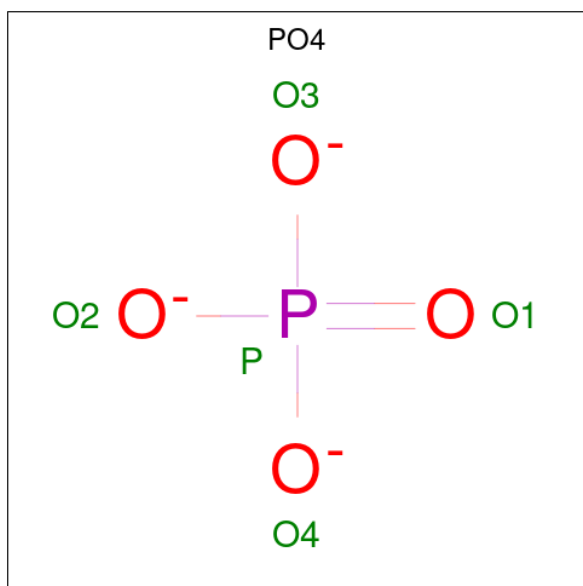
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P0C6X1
A	26	ALA	ILE	engineered mutation	UNP P0C6X1
A	52	ALA	ASN	engineered mutation	UNP P0C6X1
B	0	SER	-	expression tag	UNP P0C6X1
B	26	ALA	ILE	engineered mutation	UNP P0C6X1
B	52	ALA	ASN	engineered mutation	UNP P0C6X1
C	0	SER	-	expression tag	UNP P0C6X1
C	26	ALA	ILE	engineered mutation	UNP P0C6X1
C	52	ALA	ASN	engineered mutation	UNP P0C6X1
D	0	SER	-	expression tag	UNP P0C6X1
D	26	ALA	ILE	engineered mutation	UNP P0C6X1
D	52	ALA	ASN	engineered mutation	UNP P0C6X1
E	0	SER	-	expression tag	UNP P0C6X1
E	26	ALA	ILE	engineered mutation	UNP P0C6X1
E	52	ALA	ASN	engineered mutation	UNP P0C6X1
F	0	SER	-	expression tag	UNP P0C6X1
F	26	ALA	ILE	engineered mutation	UNP P0C6X1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	52	ALA	ASN	engineered mutation	UNP P0C6X1

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total	O	0	0
			63	63		
3	B	49	Total	O	0	0
			49	49		
3	C	102	Total	O	0	0
			102	102		

Continued on next page...

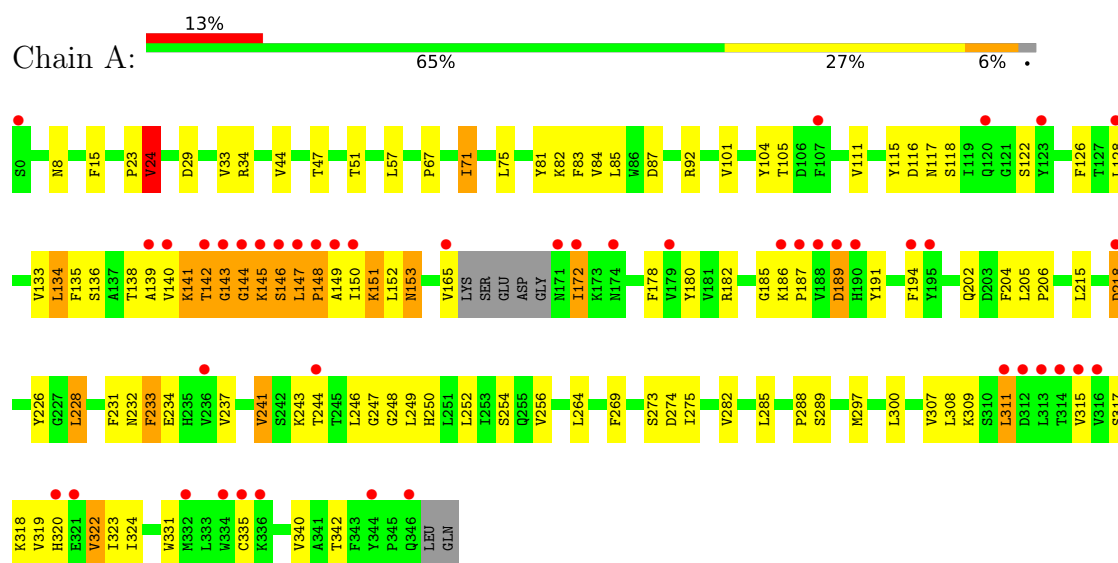
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	109	Total 109	O 109	0	0
3	E	102	Total 102	O 102	0	0
3	F	94	Total 94	O 94	0	0

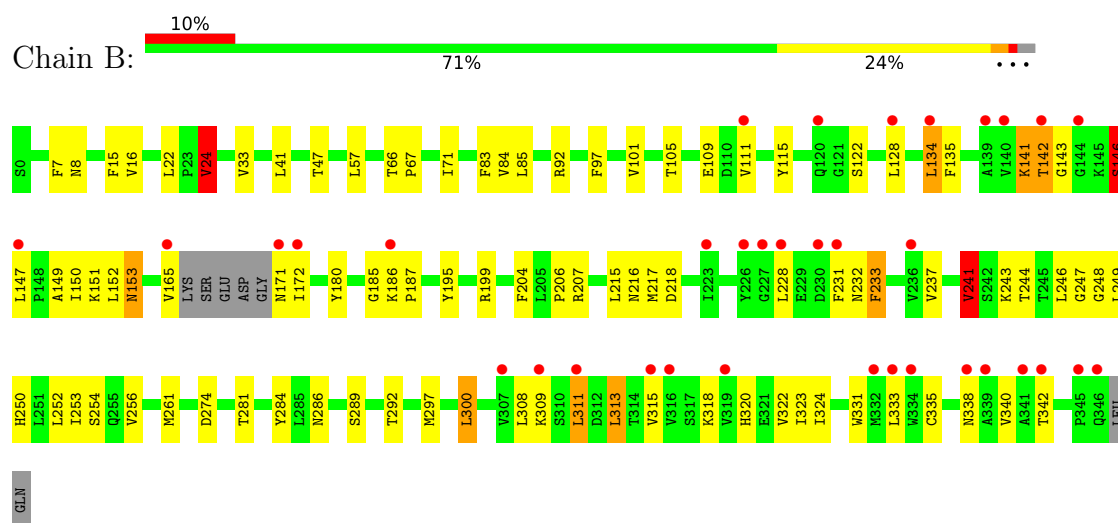
3 Residue-property plots [i](#)

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: Uridylate-specific endoribonuclease

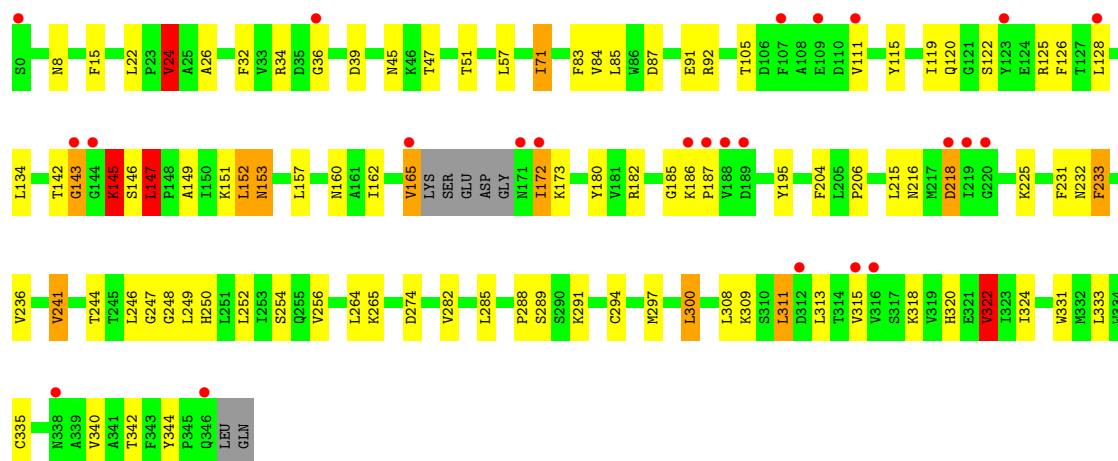


• Molecule 1: Uridylate-specific endoribonuclease

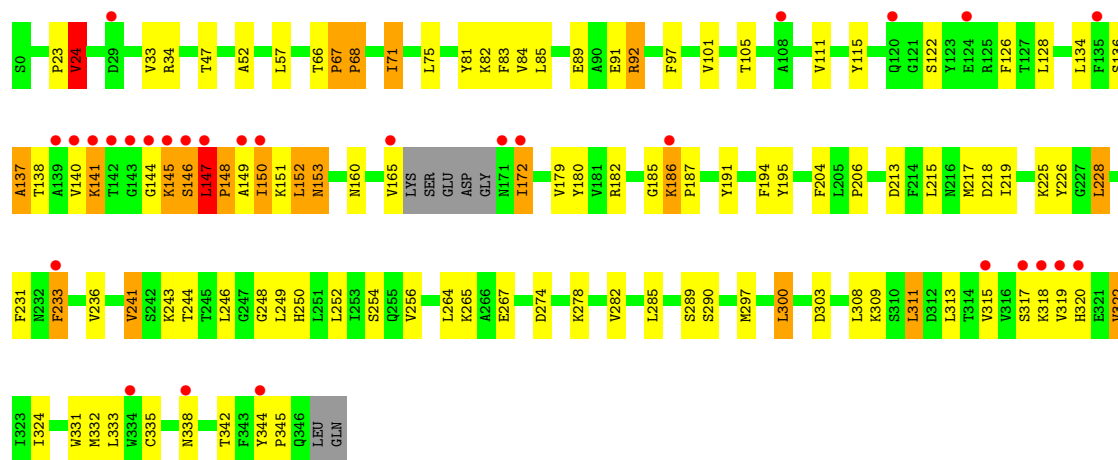


• Molecule 1: Uridylate-specific endoribonuclease

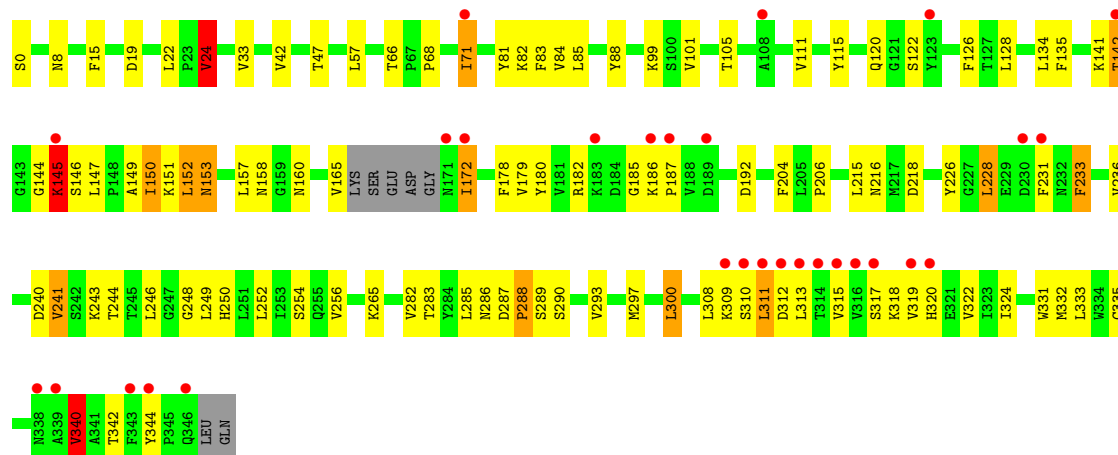




• Molecule 1: Uridylate-specific endoribonuclease

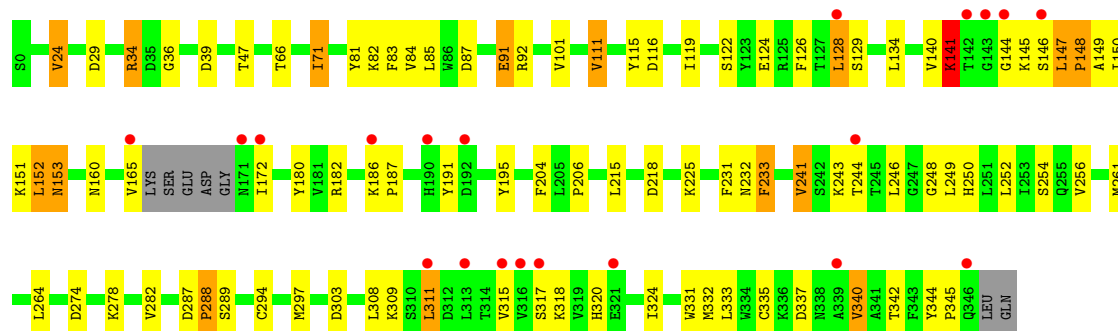


• Molecule 1: Uridylate-specific endoribonuclease



• Molecule 1: Uridylate-specific endoribonuclease

Chain F:  6% 71% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	86.44Å 140.28Å 426.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.22 – 2.50 43.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (43.22-2.50) 96.3 (43.22-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.241 , 0.285 0.239 , 0.280	Depositor DCC
R_{free} test set	4466 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtrriage
Anisotropy	0.656	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16623	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: PO4

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	1.01	2/2737 (0.1%)	1.06	6/3716 (0.2%)
1	B	1.03	1/2737 (0.0%)	1.03	9/3716 (0.2%)
1	C	0.95	1/2737 (0.0%)	1.05	8/3716 (0.2%)
1	D	0.95	0/2737	1.13	16/3716 (0.4%)
1	E	0.99	1/2737 (0.0%)	1.10	10/3716 (0.3%)
1	F	0.93	1/2737 (0.0%)	1.03	5/3716 (0.1%)
All	All	0.98	6/16422 (0.0%)	1.07	54/22296 (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	B	0	2
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	3
All	All	0	10

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	VAL	CA-CB	5.46	1.61	1.54
1	E	340	VAL	CA-CB	5.36	1.60	1.54
1	C	87	ASP	CA-C	5.25	1.59	1.52
1	B	16	VAL	CA-CB	5.16	1.61	1.54
1	F	119	ILE	CA-CB	5.04	1.60	1.54
1	A	323	ILE	CA-CB	5.00	1.59	1.53

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	ALA	CA-C-N	15.61	148.75	121.75
1	D	137	ALA	C-N-CA	15.61	148.75	121.75
1	E	172	ILE	N-CA-C	9.32	120.06	106.55
1	D	137	ALA	O-C-N	-8.74	111.03	122.39
1	A	172	ILE	N-CA-C	8.16	118.39	106.55
1	B	67	PRO	O-C-N	7.88	124.85	121.15
1	D	67	PRO	O-C-N	7.57	124.79	121.31
1	E	150	ILE	N-CA-C	-7.17	100.34	109.30
1	E	24	VAL	CB-CA-C	-7.12	98.39	110.71
1	F	24	VAL	CB-CA-C	-7.01	99.47	110.69
1	F	66	THR	CA-C-N	6.93	124.65	119.66
1	F	66	THR	C-N-CA	6.93	124.65	119.66
1	C	24	VAL	CB-CA-C	-6.75	98.63	110.71
1	D	285	LEU	N-CA-C	6.53	118.47	111.36
1	A	24	VAL	CB-CA-C	-6.41	100.64	110.50
1	D	24	VAL	CB-CA-C	-6.40	100.46	110.69
1	C	147	LEU	N-CA-C	-6.37	101.74	109.83
1	E	236	VAL	N-CA-C	6.32	117.06	110.62
1	B	24	VAL	CB-CA-C	-6.13	99.74	110.71
1	E	68	PRO	CA-C-O	-6.12	114.30	121.95
1	D	66	THR	CA-C-N	6.08	124.10	119.66
1	D	66	THR	C-N-CA	6.08	124.10	119.66
1	C	172	ILE	N-CA-C	6.07	121.97	109.34
1	D	67	PRO	CA-C-N	6.02	125.98	119.78
1	D	67	PRO	C-N-CA	6.02	125.98	119.78
1	B	101	VAL	CB-CA-C	-6.00	106.61	111.71
1	A	189	ASP	N-CA-C	5.95	118.53	111.33
1	D	68	PRO	CA-C-O	-5.82	114.81	121.56
1	C	51	THR	N-CA-C	5.70	117.49	111.28
1	B	146	SER	N-CA-C	5.58	117.46	108.32
1	E	146	SER	N-CA-C	5.53	118.24	109.50
1	C	145	LYS	N-CA-C	5.47	117.22	108.41
1	B	97	PHE	N-CA-C	5.46	118.30	109.40
1	C	26	ALA	N-CA-C	-5.45	102.42	110.48
1	D	172	ILE	N-CA-C	5.44	120.65	109.34
1	E	66	THR	CA-C-N	5.33	123.50	119.66
1	E	66	THR	C-N-CA	5.33	123.50	119.66
1	F	101	VAL	CB-CA-C	-5.33	106.37	111.44
1	B	66	THR	CA-C-N	5.32	123.49	119.66
1	B	66	THR	C-N-CA	5.32	123.49	119.66
1	A	141	LYS	N-CA-C	5.26	117.81	109.50
1	E	101	VAL	CB-CA-C	-5.25	107.25	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	VAL	N-CA-C	-5.22	107.38	112.29
1	C	236	VAL	N-CA-C	5.20	115.93	110.62
1	C	322	VAL	CB-CA-C	5.19	118.35	110.62
1	D	92	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	D	97	PHE	N-CA-C	5.12	117.74	109.40
1	E	310	SER	N-CA-C	-5.08	105.12	113.50
1	D	101	VAL	CB-CA-C	-5.07	106.63	111.44
1	B	217	MET	N-CA-C	5.06	117.06	110.53
1	A	67	PRO	O-C-N	5.05	123.53	121.15
1	D	186	LYS	N-CA-C	5.05	116.41	108.23
1	F	144	GLY	N-CA-C	-5.04	101.22	113.18
1	A	101	VAL	CB-CA-C	-5.03	106.66	111.44

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	141	LYS	Peptide
1	B	146	SER	Peptide
1	C	145	LYS	Peptide
1	C	91	GLU	Peptide
1	D	137	ALA	Peptide
1	D	91	GLU	Peptide
1	E	145	LYS	Peptide
1	F	141	LYS	Peptide
1	F	148	PRO	Peptide
1	F	91	GLU	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	2679	0	2666	135	0
1	B	2679	0	2667	65	0
1	C	2679	0	2667	73	0
1	D	2679	0	2667	115	1
1	E	2679	0	2667	80	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2679	0	2667	79	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	63	0	0	13	1
3	B	49	0	0	15	1
3	C	102	0	0	8	0
3	D	109	0	0	8	0
3	E	102	0	0	10	0
3	F	94	0	0	16	0
All	All	16623	0	16001	529	2

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 16.

All (529) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:CG1	1:A:147:LEU:HD22	1.20	1.57
1:A:140:VAL:HG11	1:A:147:LEU:CD2	1.34	1.50
1:A:143:GLY:C	1:A:145:LYS:HB3	1.33	1.48
1:D:149:ALA:HB2	1:D:180:TYR:CD1	1.61	1.32
1:A:142:THR:C	1:A:145:LYS:HB2	1.61	1.24
1:D:140:VAL:HG12	1:D:180:TYR:CZ	1.79	1.16
1:A:148:PRO:O	1:A:191:TYR:HE2	1.27	1.16
1:D:140:VAL:CG1	1:D:180:TYR:CZ	2.30	1.15
1:A:140:VAL:HG12	1:A:147:LEU:HD22	1.20	1.11
1:D:149:ALA:CB	1:D:180:TYR:CE1	2.34	1.10
1:A:144:GLY:N	1:A:145:LYS:HB3	1.69	1.06
1:D:149:ALA:CB	1:D:180:TYR:CD1	2.38	1.05
1:A:142:THR:C	1:A:145:LYS:CB	2.30	1.05
1:D:149:ALA:HB2	1:D:180:TYR:CE1	1.92	1.04
1:A:143:GLY:C	1:A:145:LYS:CB	2.30	1.04
1:B:171:ASN:ND2	3:B:502:HOH:O	1.84	1.03
1:A:140:VAL:CG1	1:A:147:LEU:CD2	2.06	1.02
1:D:140:VAL:CG1	1:D:180:TYR:CE2	2.43	1.01
1:D:150:ILE:HG21	1:D:195:TYR:OH	1.57	1.01
1:A:139:ALA:HB2	1:A:178:PHE:CE1	1.96	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ALA:HB2	1:E:180:TYR:CE1	1.96	1.00
1:A:146:SER:O	1:A:147:LEU:HB2	1.59	0.99
1:D:141:LYS:C	1:D:141:LYS:HD2	1.84	0.98
1:A:139:ALA:HB2	1:A:178:PHE:CD1	1.99	0.96
1:D:149:ALA:HA	1:D:191:TYR:CE2	2.00	0.96
1:F:231:PHE:HA	1:F:340:VAL:HG13	1.47	0.96
1:A:148:PRO:O	1:A:191:TYR:CE2	2.18	0.95
1:A:141:LYS:O	1:A:142:THR:HG22	1.66	0.95
1:A:145:LYS:O	1:A:145:LYS:HD3	1.68	0.94
1:B:149:ALA:HB2	1:B:180:TYR:CE1	2.02	0.94
1:D:140:VAL:HG12	1:D:180:TYR:CE2	2.01	0.94
1:A:269:PHE:O	3:A:513:HOH:O	1.86	0.94
1:D:150:ILE:CG2	1:D:195:TYR:OH	2.15	0.93
1:D:141:LYS:C	1:D:141:LYS:CD	2.41	0.92
1:F:297:MET:HE1	1:F:324:ILE:HD13	1.53	0.91
1:B:313:LEU:HD13	3:B:527:HOH:O	1.69	0.91
1:A:141:LYS:O	1:A:142:THR:CG2	2.17	0.91
1:A:297:MET:CE	1:A:324:ILE:HG21	2.00	0.91
1:A:134:LEU:HA	3:A:506:HOH:O	1.69	0.90
1:E:120:GLN:NE2	3:E:548:HOH:O	2.03	0.90
1:A:297:MET:HE1	1:A:324:ILE:HG21	1.54	0.90
1:A:117:ASN:HB3	1:A:136:SER:HB2	1.52	0.89
1:A:140:VAL:O	1:A:146:SER:O	1.91	0.89
1:D:140:VAL:HG12	1:D:180:TYR:OH	1.74	0.88
1:D:297:MET:HE1	1:D:324:ILE:HD13	1.58	0.86
1:D:140:VAL:HG11	1:D:180:TYR:CE2	2.08	0.86
1:D:297:MET:CE	1:D:324:ILE:HG21	2.06	0.85
1:E:297:MET:CE	1:E:324:ILE:HG21	2.08	0.84
1:E:19:ASP:OD1	3:E:576:HOH:O	1.96	0.84
1:A:140:VAL:HG11	1:A:147:LEU:HD21	1.57	0.84
1:A:149:ALA:HB2	1:A:180:TYR:CE1	2.13	0.83
1:A:318:LYS:NZ	3:A:540:HOH:O	1.98	0.83
1:A:140:VAL:O	1:A:146:SER:HA	1.78	0.82
1:A:142:THR:O	1:A:145:LYS:HB2	1.78	0.82
1:A:140:VAL:HG11	1:A:147:LEU:HD23	1.62	0.81
1:A:143:GLY:CA	1:A:145:LYS:HB3	2.10	0.81
1:F:126:PHE:O	3:F:550:HOH:O	1.98	0.81
1:A:117:ASN:CB	1:A:136:SER:HB2	2.11	0.80
1:C:249:LEU:HD12	1:C:254:SER:HB3	1.63	0.80
1:F:297:MET:CE	1:F:324:ILE:HG21	2.12	0.80
1:B:297:MET:CE	1:B:324:ILE:HG21	2.12	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:PHE:HA	1:E:340:VAL:HG13	1.63	0.79
1:A:145:LYS:O	1:A:145:LYS:CD	2.30	0.79
1:D:149:ALA:HB2	1:D:180:TYR:HD1	1.40	0.78
1:E:318:LYS:HD2	1:E:320:HIS:CE1	2.18	0.78
1:D:149:ALA:HB3	1:D:180:TYR:CE1	2.19	0.77
1:E:249:LEU:HD12	1:E:254:SER:HB3	1.67	0.77
1:A:116:ASP:OD2	3:A:512:HOH:O	2.03	0.77
1:D:149:ALA:HA	1:D:191:TYR:HE2	1.44	0.76
1:A:144:GLY:N	1:A:145:LYS:CB	2.47	0.76
1:A:143:GLY:N	1:A:145:LYS:CB	2.48	0.76
1:A:142:THR:H	1:A:145:LYS:HG2	1.50	0.75
1:E:186:LYS:HG3	1:E:187:PRO:HD2	1.69	0.75
1:D:141:LYS:HD2	1:D:141:LYS:O	1.86	0.74
1:B:297:MET:HE1	1:B:324:ILE:HD13	1.70	0.74
1:C:297:MET:HE1	1:C:324:ILE:HG21	1.68	0.74
1:E:297:MET:HE1	1:E:324:ILE:HD13	1.70	0.73
1:C:297:MET:CE	1:C:324:ILE:HG21	2.18	0.73
1:A:141:LYS:C	1:A:142:THR:HG23	2.13	0.73
1:E:297:MET:HE1	1:E:324:ILE:HG21	1.71	0.73
1:D:297:MET:HE1	1:D:324:ILE:HG21	1.70	0.73
1:A:133:VAL:O	3:A:506:HOH:O	2.06	0.72
1:A:141:LYS:C	1:A:142:THR:CG2	2.61	0.72
1:C:149:ALA:HB2	1:C:180:TYR:CE1	2.23	0.72
1:D:318:LYS:HD2	1:D:320:HIS:CE1	2.25	0.71
1:A:275:ILE:HA	3:A:546:HOH:O	1.90	0.70
1:F:318:LYS:HD2	1:F:320:HIS:CE1	2.26	0.70
1:A:140:VAL:CB	1:A:147:LEU:HD22	2.17	0.70
1:F:303:ASP:OD2	3:F:505:HOH:O	2.09	0.70
1:D:147:LEU:O	1:D:148:PRO:O	2.09	0.70
1:A:218:ASP:OD1	1:D:225:LYS:HE2	1.91	0.70
1:F:278:LYS:HE3	3:F:537:HOH:O	1.92	0.69
1:D:267:GLU:OE2	3:D:582:HOH:O	2.10	0.69
1:A:218:ASP:OD1	1:D:225:LYS:CE	2.39	0.69
1:B:297:MET:HE1	1:B:324:ILE:HG21	1.72	0.69
1:D:249:LEU:HD12	1:D:254:SER:HB3	1.74	0.69
1:D:144:GLY:O	1:D:145:LYS:CB	2.40	0.68
1:E:192:ASP:O	3:E:564:HOH:O	2.11	0.68
1:A:146:SER:O	1:A:147:LEU:CB	2.36	0.68
1:E:293:VAL:O	3:E:554:HOH:O	2.12	0.68
1:E:158:ASN:O	3:E:507:HOH:O	2.12	0.67
1:A:115:TYR:N	3:A:506:HOH:O	2.23	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:O	1:A:148:PRO:C	2.37	0.67
1:E:311:LEU:CD1	1:E:320:HIS:HD2	2.08	0.67
1:A:143:GLY:O	1:A:145:LYS:HB3	1.91	0.67
1:C:125:ARG:NH1	3:C:511:HOH:O	2.18	0.67
1:F:311:LEU:CD1	1:F:320:HIS:HD2	2.07	0.66
1:A:246:LEU:HB2	1:A:289:SER:OG	1.95	0.66
1:D:92:ARG:NH2	3:D:575:HOH:O	2.28	0.65
1:E:149:ALA:CB	1:E:180:TYR:CE1	2.78	0.65
1:F:337:ASP:OD2	3:F:561:HOH:O	2.14	0.65
1:D:315:VAL:O	1:D:335:CYS:HB2	1.96	0.65
2:C:401:PO4:O1	3:C:504:HOH:O	2.15	0.65
1:B:246:LEU:HB2	1:B:289:SER:OG	1.96	0.65
1:C:45:ASN:O	3:C:519:HOH:O	2.14	0.65
1:C:318:LYS:HD2	1:C:320:HIS:CE1	2.32	0.65
1:D:146:SER:O	1:D:147:LEU:C	2.39	0.65
1:C:173:LYS:NZ	1:E:241:VAL:O	2.30	0.65
1:A:142:THR:H	1:A:145:LYS:CG	2.09	0.65
1:A:142:THR:O	1:A:144:GLY:N	2.30	0.64
1:E:153:ASN:H	1:E:153:ASN:HD22	1.44	0.64
1:A:145:LYS:HD2	1:A:145:LYS:N	2.12	0.64
1:A:186:LYS:HG3	1:A:187:PRO:HD2	1.80	0.64
1:E:115:TYR:HB3	1:E:122:SER:HB3	1.80	0.64
1:E:240:ASP:O	3:E:585:HOH:O	2.15	0.64
1:A:118:SER:OG	3:A:539:HOH:O	2.14	0.64
1:D:149:ALA:CA	1:D:191:TYR:CE2	2.79	0.64
1:F:297:MET:HE3	1:F:324:ILE:HG21	1.80	0.64
1:D:148:PRO:O	1:D:149:ALA:HB3	1.98	0.63
1:E:315:VAL:O	1:E:335:CYS:HB2	1.99	0.63
1:F:249:LEU:HD12	1:F:254:SER:HB3	1.81	0.63
1:A:140:VAL:O	1:A:146:SER:CA	2.47	0.63
1:A:143:GLY:N	1:A:145:LYS:HG3	2.13	0.62
1:D:150:ILE:HG23	1:D:191:TYR:CB	2.30	0.62
1:C:92:ARG:NH1	1:C:274:ASP:OD2	2.30	0.62
1:E:83:PHE:HE1	1:E:85:LEU:HG	1.64	0.62
1:F:153:ASN:HD22	1:F:153:ASN:H	1.47	0.62
1:A:142:THR:O	1:A:145:LYS:CB	2.44	0.62
1:D:186:LYS:HG3	1:D:187:PRO:HD2	1.82	0.62
1:B:308:LEU:HA	1:B:311:LEU:HD22	1.82	0.62
1:A:142:THR:CA	1:A:145:LYS:HB2	2.29	0.62
1:F:308:LEU:HA	1:F:311:LEU:HD22	1.82	0.62
1:A:308:LEU:HA	1:A:311:LEU:HD22	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:GLY:O	1:D:145:LYS:HB3	2.00	0.61
1:B:204:PHE:CG	1:B:256:VAL:HG21	2.34	0.61
1:B:318:LYS:HD2	1:B:320:HIS:CE1	2.35	0.61
1:A:315:VAL:O	1:A:335:CYS:HB2	2.00	0.61
1:B:249:LEU:HD12	1:B:254:SER:HB3	1.81	0.61
1:A:143:GLY:O	1:A:144:GLY:C	2.44	0.61
1:B:315:VAL:O	1:B:335:CYS:HB2	2.01	0.61
1:D:149:ALA:CA	1:D:191:TYR:HE2	2.14	0.60
1:B:313:LEU:N	3:B:527:HOH:O	2.34	0.60
1:D:153:ASN:HD22	1:D:153:ASN:H	1.49	0.60
1:D:219:ILE:HG13	3:D:605:HOH:O	2.01	0.60
1:D:308:LEU:HA	1:D:311:LEU:HD22	1.83	0.60
1:D:322:VAL:HG13	1:D:331:TRP:CD1	2.36	0.60
1:D:52:ALA:O	3:D:502:HOH:O	2.17	0.60
1:D:144:GLY:O	1:D:145:LYS:CG	2.49	0.60
1:E:149:ALA:HB2	1:E:180:TYR:HE1	1.62	0.60
1:A:115:TYR:O	3:A:506:HOH:O	2.16	0.60
1:A:153:ASN:HD22	1:A:153:ASN:H	1.51	0.59
1:C:153:ASN:H	1:C:153:ASN:HD22	1.50	0.59
1:E:308:LEU:HA	1:E:311:LEU:HD22	1.85	0.59
1:F:150:ILE:HG23	1:F:195:TYR:OH	2.02	0.59
1:B:253:ILE:HB	3:B:506:HOH:O	2.01	0.59
1:B:41:LEU:O	3:B:504:HOH:O	2.15	0.59
1:F:186:LYS:CE	3:F:559:HOH:O	2.51	0.59
1:C:186:LYS:HG3	1:C:187:PRO:HD2	1.84	0.58
1:F:91:GLU:HG2	3:F:543:HOH:O	2.03	0.58
1:D:150:ILE:HG23	1:D:191:TYR:HB2	1.85	0.58
1:B:311:LEU:HD12	1:B:320:HIS:HD2	1.67	0.58
1:C:297:MET:HE1	1:C:324:ILE:HD13	1.86	0.58
1:C:311:LEU:CD1	1:C:320:HIS:HD2	2.15	0.58
1:F:297:MET:HE1	1:F:324:ILE:HG21	1.84	0.58
1:B:311:LEU:CD1	1:B:320:HIS:HD2	2.17	0.58
1:C:231:PHE:O	1:C:233:PHE:N	2.36	0.58
1:C:83:PHE:HE1	1:C:85:LEU:HG	1.67	0.58
1:E:150:ILE:HB	1:E:179:VAL:HB	1.86	0.58
1:E:297:MET:HE3	1:E:324:ILE:HG21	1.85	0.58
1:A:297:MET:HE1	1:A:324:ILE:HD13	1.85	0.58
1:C:160:ASN:OD1	1:E:265:LYS:HG3	2.03	0.58
1:B:115:TYR:HB3	1:B:122:SER:HB3	1.86	0.58
1:D:136:SER:OG	1:D:138:THR:HG22	2.04	0.58
1:A:249:LEU:HD12	1:A:254:SER:HB3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:PHE:CG	1:D:256:VAL:HG21	2.39	0.57
1:A:140:VAL:O	1:A:146:SER:C	2.47	0.57
1:F:186:LYS:HG3	1:F:187:PRO:HD2	1.84	0.57
1:F:297:MET:HE1	1:F:324:ILE:CD1	2.32	0.57
1:B:92:ARG:NH1	1:B:274:ASP:OD2	2.32	0.57
1:C:308:LEU:HA	1:C:311:LEU:HD22	1.85	0.57
1:A:115:TYR:HB3	1:A:122:SER:HB3	1.85	0.57
1:C:311:LEU:HD12	1:C:320:HIS:HD2	1.70	0.57
1:C:115:TYR:HB3	1:C:122:SER:HB3	1.86	0.57
1:F:246:LEU:HB2	1:F:289:SER:OG	2.04	0.56
1:A:143:GLY:N	1:A:145:LYS:HB3	2.19	0.56
1:D:89:GLU:O	3:D:513:HOH:O	2.17	0.56
1:D:297:MET:HE3	1:D:324:ILE:HG21	1.87	0.56
1:D:311:LEU:CD1	1:D:320:HIS:HD2	2.18	0.56
1:A:142:THR:H	1:A:145:LYS:HB2	1.71	0.56
1:F:204:PHE:CG	1:F:256:VAL:HG21	2.40	0.56
1:D:115:TYR:HB3	1:D:122:SER:HB3	1.88	0.56
1:B:153:ASN:HD22	1:B:153:ASN:H	1.53	0.56
1:A:143:GLY:N	1:A:145:LYS:CG	2.68	0.56
1:D:144:GLY:C	1:D:145:LYS:HG2	2.30	0.56
1:E:57:LEU:HD11	1:E:105:THR:HG21	1.86	0.56
1:E:248:GLY:C	1:E:250:HIS:HD2	2.15	0.55
1:A:142:THR:H	1:A:145:LYS:CB	2.19	0.55
1:A:104:TYR:HB2	3:A:509:HOH:O	2.07	0.55
1:A:311:LEU:CD1	1:A:320:HIS:HD2	2.19	0.55
1:C:225:LYS:NZ	3:C:523:HOH:O	2.32	0.55
1:F:206:PRO:HG3	1:F:215:LEU:HD12	1.88	0.55
1:A:57:LEU:HD11	1:A:105:THR:HG21	1.88	0.54
1:A:142:THR:N	1:A:145:LYS:HG2	2.19	0.54
1:B:286:ASN:HA	3:B:513:HOH:O	2.07	0.54
1:F:248:GLY:C	1:F:250:HIS:HD2	2.15	0.54
1:C:157:LEU:HD21	1:E:290:SER:HB3	1.90	0.54
1:B:83:PHE:HE1	1:B:85:LEU:HG	1.73	0.54
1:A:231:PHE:O	1:A:233:PHE:N	2.40	0.54
1:D:231:PHE:O	1:D:233:PHE:N	2.39	0.54
1:F:231:PHE:O	1:F:233:PHE:N	2.40	0.54
1:A:83:PHE:HE1	1:A:85:LEU:HG	1.72	0.54
1:B:186:LYS:HG3	1:B:187:PRO:HD2	1.90	0.54
1:D:140:VAL:O	1:D:141:LYS:HB3	2.07	0.53
1:D:322:VAL:CG1	1:D:331:TRP:CD1	2.92	0.53
1:D:278:LYS:NZ	3:D:512:HOH:O	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:LEU:HD12	1:E:320:HIS:HD2	1.73	0.53
1:C:241:VAL:O	1:C:241:VAL:HG13	2.08	0.53
1:C:311:LEU:HD12	1:C:320:HIS:CD2	2.43	0.53
1:E:81:TYR:CE2	1:E:82:LYS:HG3	2.43	0.53
1:A:218:ASP:OD1	1:D:225:LYS:HE3	2.09	0.53
1:D:83:PHE:HE1	1:D:85:LEU:HG	1.74	0.53
1:F:141:LYS:HA	1:F:146:SER:HA	1.91	0.53
1:A:135:PHE:HA	1:A:178:PHE:O	2.09	0.53
1:D:57:LEU:HD11	1:D:105:THR:HG21	1.91	0.53
1:B:311:LEU:HD12	1:B:320:HIS:CD2	2.43	0.53
1:B:311:LEU:O	3:B:527:HOH:O	2.19	0.53
1:E:311:LEU:HG	1:E:333:LEU:HD22	1.90	0.53
1:C:322:VAL:HG13	1:C:331:TRP:CD1	2.43	0.53
1:F:115:TYR:HB3	1:F:122:SER:HB3	1.91	0.53
1:A:273:SER:O	3:A:544:HOH:O	2.19	0.53
1:F:311:LEU:HD12	1:F:320:HIS:HD2	1.72	0.52
1:F:315:VAL:O	1:F:335:CYS:HB2	2.09	0.52
1:A:142:THR:N	1:A:145:LYS:HB2	2.24	0.52
1:C:315:VAL:O	1:C:335:CYS:HB2	2.09	0.52
1:D:141:LYS:HD2	1:D:141:LYS:N	2.22	0.52
1:F:83:PHE:HE1	1:F:85:LEU:HG	1.75	0.52
1:C:157:LEU:HG	1:E:283:THR:HG23	1.92	0.52
1:F:150:ILE:HG12	1:F:191:TYR:CG	2.45	0.52
1:A:138:THR:HG22	1:A:139:ALA:N	2.25	0.52
1:C:160:ASN:HB3	1:E:285:LEU:HD11	1.90	0.52
1:D:311:LEU:HD12	1:D:320:HIS:HD2	1.74	0.52
1:A:126:PHE:CZ	1:A:182:ARG:HG3	2.45	0.52
1:D:141:LYS:HA	1:D:147:LEU:HD12	1.91	0.52
1:F:311:LEU:HD12	1:F:320:HIS:CD2	2.45	0.52
1:D:225:LYS:NZ	3:D:553:HOH:O	2.24	0.52
1:B:311:LEU:C	3:B:527:HOH:O	2.53	0.51
1:B:109:GLU:HB2	3:B:525:HOH:O	2.09	0.51
1:D:241:VAL:O	1:D:241:VAL:HG13	2.10	0.51
1:D:231:PHE:CZ	1:D:309:LYS:HG2	2.45	0.51
1:F:241:VAL:O	1:F:241:VAL:HG13	2.10	0.51
1:B:231:PHE:CZ	1:B:309:LYS:HG2	2.46	0.51
1:D:246:LEU:HB2	1:D:289:SER:OG	2.11	0.51
1:D:92:ARG:NH1	1:D:274:ASP:OD2	2.32	0.51
1:E:88:TYR:OH	3:E:528:HOH:O	2.14	0.51
1:A:231:PHE:CZ	1:A:309:LYS:HG2	2.46	0.51
1:B:149:ALA:HB2	1:B:180:TYR:CZ	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:VAL:HG22	1:F:289:SER:HB3	1.92	0.51
1:E:204:PHE:CG	1:E:256:VAL:HG21	2.46	0.50
1:B:24:VAL:HG13	1:B:33:VAL:HG22	1.92	0.50
1:E:231:PHE:CZ	1:E:309:LYS:HG2	2.46	0.50
1:F:124:GLU:O	1:F:128:LEU:HD22	2.12	0.50
1:D:248:GLY:C	1:D:250:HIS:HD2	2.20	0.50
1:E:311:LEU:HD12	1:E:320:HIS:CD2	2.47	0.50
1:A:140:VAL:N	1:A:180:TYR:OH	2.39	0.50
1:A:322:VAL:HG13	1:A:331:TRP:CD1	2.47	0.50
1:C:248:GLY:C	1:C:250:HIS:HD2	2.20	0.50
1:D:71:ILE:CD1	1:D:152:LEU:HD21	2.42	0.50
1:E:153:ASN:HD22	1:E:153:ASN:N	2.06	0.50
1:D:194:PHE:CD2	1:D:303:ASP:HB3	2.46	0.50
1:A:140:VAL:HG12	1:A:147:LEU:CD2	2.11	0.49
1:B:153:ASN:HD22	1:B:153:ASN:N	2.10	0.49
1:F:126:PHE:CZ	1:F:182:ARG:HG3	2.47	0.49
1:A:297:MET:HE3	1:A:324:ILE:HG21	1.91	0.49
1:E:249:LEU:CD1	1:E:254:SER:HB3	2.41	0.49
1:A:139:ALA:CB	1:A:178:PHE:CD1	2.86	0.49
1:D:311:LEU:HG	1:D:333:LEU:HD22	1.95	0.49
1:F:186:LYS:NZ	3:F:559:HOH:O	2.39	0.49
1:C:322:VAL:HG22	1:C:324:ILE:HD11	1.95	0.49
1:A:151:LYS:HE3	1:A:151:LYS:H	1.78	0.48
1:C:265:LYS:HG3	1:D:160:ASN:OD1	2.12	0.48
1:B:216:ASN:N	1:B:216:ASN:HD22	2.09	0.48
1:F:92:ARG:NH1	1:F:274:ASP:OD2	2.42	0.48
1:F:141:LYS:HE2	1:F:146:SER:HB3	1.96	0.48
1:C:57:LEU:HD11	1:C:105:THR:HG21	1.96	0.48
1:E:8:ASN:HB3	1:E:15:PHE:HA	1.95	0.48
1:D:150:ILE:HG13	1:D:179:VAL:O	2.13	0.48
1:E:231:PHE:CE2	1:E:309:LYS:HG2	2.48	0.48
1:F:182:ARG:NE	3:F:550:HOH:O	2.46	0.48
1:B:187:PRO:HB3	3:B:536:HOH:O	2.12	0.48
1:F:231:PHE:CZ	1:F:309:LYS:HG2	2.49	0.48
1:A:297:MET:HE1	1:A:324:ILE:CG2	2.35	0.48
1:C:34:ARG:HD3	1:C:39:ASP:OD1	2.14	0.48
1:A:147:LEU:O	1:A:180:TYR:HE1	1.96	0.48
1:F:149:ALA:HB2	1:F:180:TYR:CE1	2.49	0.48
1:D:250:HIS:CE1	1:D:344:TYR:CB	2.97	0.47
1:E:318:LYS:HD2	1:E:320:HIS:HE1	1.72	0.47
1:C:311:LEU:CD1	1:C:320:HIS:CD2	2.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:HIS:CE1	1:D:344:TYR:HB2	2.49	0.47
1:D:250:HIS:HD1	1:D:345:PRO:HD2	1.79	0.47
1:E:206:PRO:HG3	1:E:215:LEU:HD12	1.96	0.47
1:C:24:VAL:HA	1:C:32:PHE:O	2.13	0.47
1:C:204:PHE:CG	1:C:256:VAL:HG21	2.49	0.47
1:B:231:PHE:CE2	1:B:309:LYS:HG2	2.49	0.47
1:E:42:VAL:O	3:E:597:HOH:O	2.20	0.47
1:A:23:PRO:HB2	1:A:34:ARG:HB2	1.96	0.47
1:E:318:LYS:HD2	1:E:320:HIS:ND1	2.30	0.47
1:F:92:ARG:NH2	3:F:511:HOH:O	2.47	0.47
1:A:148:PRO:CG	1:A:189:ASP:O	2.63	0.47
1:B:134:LEU:HD22	1:B:135:PHE:N	2.30	0.47
1:B:253:ILE:N	3:B:506:HOH:O	2.12	0.47
1:C:153:ASN:HD22	1:C:153:ASN:N	2.10	0.47
1:E:250:HIS:CE1	1:E:344:TYR:CB	2.98	0.47
1:A:92:ARG:NH1	1:A:274:ASP:OD2	2.44	0.47
1:B:57:LEU:HD11	1:B:105:THR:HG21	1.97	0.47
1:B:313:LEU:CD1	3:B:527:HOH:O	2.45	0.47
1:E:135:PHE:HA	1:E:178:PHE:O	2.15	0.46
1:E:248:GLY:C	1:E:250:HIS:CD2	2.93	0.46
1:F:29:ASP:HB3	3:F:574:HOH:O	2.15	0.46
1:F:81:TYR:CE2	1:F:82:LYS:HG3	2.50	0.46
1:D:141:LYS:C	1:D:141:LYS:HD3	2.36	0.46
1:E:246:LEU:HB2	1:E:289:SER:OG	2.14	0.46
1:F:147:LEU:HD22	1:F:148:PRO:HD2	1.97	0.46
1:E:71:ILE:CD1	1:E:152:LEU:HD21	2.46	0.46
1:C:232:ASN:H	1:C:340:VAL:HB	1.79	0.46
1:C:248:GLY:C	1:C:250:HIS:CD2	2.94	0.46
1:C:311:LEU:HG	1:C:333:LEU:HD22	1.97	0.46
1:D:148:PRO:O	1:D:149:ALA:CB	2.64	0.46
1:D:311:LEU:HD12	1:D:320:HIS:CD2	2.50	0.46
1:E:81:TYR:OH	1:E:82:LYS:HE3	2.15	0.46
1:C:218:ASP:OD1	1:F:225:LYS:CE	2.64	0.46
1:A:194:PHE:O	1:A:324:ILE:HA	2.16	0.46
1:C:147:LEU:HD22	1:C:147:LEU:HA	1.76	0.46
1:F:297:MET:CE	1:F:324:ILE:HD13	2.36	0.46
1:B:215:LEU:C	1:B:216:ASN:HD22	2.24	0.46
1:C:119:ILE:O	1:C:120:GLN:C	2.59	0.46
1:C:247:GLY:HA2	3:C:504:HOH:O	2.15	0.46
1:E:0:SER:N	3:E:563:HOH:O	2.48	0.46
1:B:248:GLY:C	1:B:250:HIS:CD2	2.94	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:MET:HE3	1:B:324:ILE:HG21	1.95	0.46
1:D:126:PHE:CZ	1:D:182:ARG:HG3	2.51	0.46
1:A:142:THR:O	1:A:142:THR:OG1	2.30	0.46
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.83	0.46
1:E:250:HIS:CE1	1:E:344:TYR:HB2	2.51	0.46
1:F:150:ILE:HG23	1:F:195:TYR:CZ	2.51	0.45
1:A:151:LYS:HG3	1:A:178:PHE:CE1	2.52	0.45
1:C:215:LEU:C	1:C:216:ASN:HD22	2.24	0.45
1:D:140:VAL:HG13	1:D:180:TYR:CZ	2.42	0.45
1:F:111:VAL:HG22	3:F:545:HOH:O	2.17	0.45
1:E:149:ALA:HB2	1:E:180:TYR:CZ	2.48	0.45
1:F:232:ASN:HB2	1:F:340:VAL:O	2.16	0.45
1:A:134:LEU:HD22	1:A:135:PHE:N	2.31	0.45
1:B:150:ILE:HG23	1:B:195:TYR:CZ	2.51	0.45
1:F:146:SER:O	1:F:147:LEU:HD23	2.16	0.45
1:F:248:GLY:C	1:F:250:HIS:CD2	2.94	0.45
1:D:144:GLY:C	1:D:145:LYS:CG	2.88	0.45
1:D:264:LEU:HD11	1:D:282:VAL:CG2	2.46	0.45
1:E:126:PHE:CZ	1:E:182:ARG:HG3	2.52	0.45
1:D:185:GLY:O	1:D:186:LYS:HD2	2.17	0.45
1:A:232:ASN:H	1:A:340:VAL:HB	1.82	0.45
1:B:206:PRO:HG3	1:B:215:LEU:HD12	1.99	0.45
1:D:206:PRO:HG3	1:D:215:LEU:HD12	1.99	0.45
1:D:317:SER:HB2	1:D:332:MET:HE1	1.98	0.45
1:D:231:PHE:CE2	1:D:309:LYS:HG2	2.51	0.45
1:E:226:TYR:O	1:E:228:LEU:HD13	2.17	0.44
1:E:231:PHE:O	1:E:233:PHE:N	2.47	0.44
1:E:300:LEU:HD23	1:E:300:LEU:HA	1.78	0.44
1:F:318:LYS:HD2	1:F:320:HIS:HE1	1.81	0.44
1:F:331:TRP:CZ3	1:F:345:PRO:HD3	2.52	0.44
1:C:231:PHE:CZ	1:C:309:LYS:HG2	2.52	0.44
1:F:231:PHE:HA	1:F:340:VAL:CG1	2.33	0.44
1:A:206:PRO:HG3	1:A:215:LEU:HD12	1.99	0.44
1:B:185:GLY:O	1:B:186:LYS:HD2	2.17	0.44
1:D:147:LEU:O	1:D:148:PRO:C	2.59	0.44
1:D:318:LYS:HD2	1:D:320:HIS:ND1	2.32	0.44
1:E:22:LEU:O	1:E:24:VAL:HG22	2.16	0.44
1:A:71:ILE:O	1:A:75:LEU:HG	2.17	0.44
1:C:216:ASN:HD22	1:C:216:ASN:N	2.13	0.44
1:D:23:PRO:HB2	1:D:34:ARG:HB2	2.00	0.44
1:A:311:LEU:HD12	1:A:320:HIS:HD2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG22	1:A:324:ILE:HD11	2.00	0.44
1:D:150:ILE:HG22	1:D:195:TYR:OH	2.09	0.44
1:D:248:GLY:C	1:D:250:HIS:CD2	2.95	0.44
1:B:248:GLY:C	1:B:250:HIS:HD2	2.26	0.44
1:B:313:LEU:O	1:B:338:ASN:HA	2.17	0.44
1:C:157:LEU:HD11	1:E:290:SER:OG	2.17	0.44
1:D:213:ASP:CG	1:D:217:MET:HE3	2.42	0.44
1:A:204:PHE:CG	1:A:256:VAL:HG21	2.53	0.44
1:F:71:ILE:CD1	1:F:152:LEU:HD21	2.48	0.44
1:F:294:CYS:HA	3:F:506:HOH:O	2.18	0.44
1:A:147:LEU:O	1:A:180:TYR:CE1	2.71	0.44
1:A:248:GLY:C	1:A:250:HIS:HD2	2.25	0.44
1:B:253:ILE:CB	3:B:506:HOH:O	2.63	0.44
1:E:243:LYS:HE2	1:E:243:LYS:HB2	1.86	0.44
1:F:116:ASP:OD1	1:F:116:ASP:C	2.61	0.44
1:F:261:MET:HE3	1:F:261:MET:HB3	1.86	0.44
1:B:232:ASN:HB2	1:B:340:VAL:O	2.18	0.43
1:C:92:ARG:NH2	3:C:600:HOH:O	2.51	0.43
1:D:243:LYS:HE2	1:D:243:LYS:HB2	1.84	0.43
1:D:249:LEU:CD1	1:D:254:SER:HB3	2.46	0.43
1:E:322:VAL:HG23	1:E:331:TRP:CD1	2.53	0.43
1:A:234:GLU:HB2	3:A:550:HOH:O	2.18	0.43
1:A:317:SER:CB	3:A:534:HOH:O	2.65	0.43
1:C:162:ILE:HB	1:E:288:PRO:HG3	2.00	0.43
1:A:185:GLY:O	1:A:186:LYS:HD2	2.18	0.43
1:B:199:ARG:CZ	1:B:204:PHE:CE1	3.01	0.43
1:A:243:LYS:HB2	1:A:243:LYS:HE2	1.79	0.43
1:C:22:LEU:O	1:C:24:VAL:HG22	2.18	0.43
1:D:150:ILE:HG23	1:D:191:TYR:HB3	2.00	0.43
1:D:81:TYR:CE2	1:D:82:LYS:HG3	2.53	0.43
1:F:243:LYS:NZ	3:F:589:HOH:O	2.46	0.43
1:A:202:GLN:CD	1:A:202:GLN:H	2.27	0.43
1:B:237:VAL:O	1:B:254:SER:HB3	2.19	0.43
1:B:323:ILE:C	1:B:324:ILE:HG13	2.43	0.43
1:C:250:HIS:CE1	1:C:344:TYR:HB2	2.54	0.43
1:F:243:LYS:HB2	1:F:243:LYS:HE2	1.81	0.43
1:F:250:HIS:CE1	1:F:344:TYR:CB	3.01	0.43
1:A:264:LEU:HD11	1:A:282:VAL:CG2	2.49	0.43
1:D:24:VAL:HG13	1:D:33:VAL:HG22	2.00	0.43
1:E:250:HIS:CE1	1:E:344:TYR:HB3	2.54	0.43
1:F:160:ASN:OD1	3:F:591:HOH:O	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ASN:HB3	1:B:15:PHE:HA	2.00	0.43
1:C:206:PRO:HG3	1:C:215:LEU:HD12	2.01	0.43
1:F:250:HIS:CE1	1:F:344:TYR:HB2	2.54	0.43
1:A:141:LYS:O	1:A:142:THR:HG23	2.01	0.42
1:B:261:MET:HB3	1:B:261:MET:HE3	1.87	0.42
1:C:218:ASP:OD1	1:F:225:LYS:HE3	2.19	0.42
1:C:264:LEU:HD11	1:C:282:VAL:CG2	2.49	0.42
1:D:146:SER:O	1:D:148:PRO:N	2.52	0.42
1:E:282:VAL:O	1:E:290:SER:HA	2.18	0.42
1:B:311:LEU:HG	1:B:333:LEU:HD22	2.01	0.42
1:F:311:LEU:HG	1:F:333:LEU:HD22	2.01	0.42
1:A:318:LYS:HG2	1:A:319:VAL:N	2.34	0.42
1:A:145:LYS:CD	1:A:145:LYS:C	2.90	0.42
1:B:243:LYS:HB2	1:B:243:LYS:HE2	1.85	0.42
1:B:311:LEU:CD1	1:B:320:HIS:CD2	2.99	0.42
1:C:8:ASN:HB3	1:C:15:PHE:HA	2.02	0.42
1:C:153:ASN:C	1:C:153:ASN:ND2	2.78	0.42
1:D:300:LEU:HD23	1:D:300:LEU:HA	1.93	0.42
1:E:318:LYS:HG2	1:E:319:VAL:N	2.35	0.42
1:F:182:ARG:HD3	3:F:550:HOH:O	2.20	0.42
1:C:143:GLY:C	1:C:145:LYS:H	2.28	0.42
1:C:250:HIS:CE1	1:C:344:TYR:CB	3.02	0.42
1:E:99:LYS:NZ	3:E:557:HOH:O	2.53	0.42
1:D:322:VAL:HG22	1:D:324:ILE:HD11	2.01	0.42
1:F:318:LYS:HD2	1:F:320:HIS:ND1	2.34	0.42
1:C:165:VAL:HG21	1:E:286:ASN:O	2.19	0.42
1:C:246:LEU:HB2	1:C:289:SER:OG	2.19	0.42
1:D:226:TYR:O	1:D:228:LEU:HD13	2.19	0.42
1:D:250:HIS:CE1	1:D:344:TYR:HB3	2.54	0.42
1:E:24:VAL:HG13	1:E:33:VAL:HG22	2.02	0.42
1:E:142:THR:HG23	1:E:145:LYS:C	2.45	0.42
1:A:142:THR:N	1:A:145:LYS:CG	2.81	0.42
1:C:195:TYR:HB3	3:C:532:HOH:O	2.19	0.42
1:A:148:PRO:HG2	1:A:189:ASP:O	2.20	0.42
1:A:226:TYR:O	1:A:228:LEU:HD13	2.20	0.42
1:D:140:VAL:HG11	1:D:180:TYR:CD2	2.53	0.42
1:F:34:ARG:HD3	1:F:39:ASP:OD1	2.19	0.42
1:A:81:TYR:CE2	1:A:82:LYS:HG3	2.55	0.42
1:B:231:PHE:O	1:B:233:PHE:N	2.48	0.42
1:D:71:ILE:O	1:D:75:LEU:HG	2.19	0.42
1:F:231:PHE:CE2	1:F:309:LYS:HG2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASN:HB2	1:A:340:VAL:O	2.19	0.41
1:A:29:ASP:HA	1:A:51:THR:OG1	2.21	0.41
1:D:236:VAL:HG22	3:D:581:HOH:O	2.19	0.41
1:D:265:LYS:HG3	1:E:160:ASN:OD1	2.20	0.41
1:E:215:LEU:C	1:E:216:ASN:HD22	2.29	0.41
1:C:185:GLY:O	1:C:186:LYS:HD2	2.21	0.41
1:D:140:VAL:HG22	1:D:147:LEU:HD13	2.03	0.41
1:D:311:LEU:CD1	1:D:320:HIS:CD2	3.03	0.41
1:A:318:LYS:HE3	1:A:320:HIS:HE1	1.85	0.41
1:C:71:ILE:CD1	1:C:152:LEU:HD21	2.51	0.41
1:D:318:LYS:HG2	1:D:319:VAL:N	2.36	0.41
1:B:241:VAL:O	1:B:241:VAL:HG13	2.20	0.41
1:C:173:LYS:NZ	1:E:287:ASP:OD1	2.53	0.41
1:C:322:VAL:HG22	1:C:324:ILE:CD1	2.51	0.41
1:E:185:GLY:O	1:E:186:LYS:HD2	2.21	0.41
1:F:87:ASP:OD1	1:F:87:ASP:C	2.63	0.41
1:A:311:LEU:HD12	1:A:320:HIS:CD2	2.56	0.41
1:C:248:GLY:HA2	3:C:591:HOH:O	2.20	0.41
1:C:291:LYS:HD3	1:C:294:CYS:HA	2.02	0.41
1:F:129:SER:HB2	3:F:550:HOH:O	2.19	0.41
1:F:317:SER:HB2	1:F:332:MET:HE1	2.03	0.41
1:A:231:PHE:CE2	1:A:309:LYS:HG2	2.55	0.41
1:B:247:GLY:HA2	3:B:538:HOH:O	2.21	0.41
1:F:287:ASP:O	1:F:288:PRO:C	2.64	0.41
1:A:246:LEU:HD12	1:A:247:GLY:N	2.36	0.41
1:A:285:LEU:N	1:A:285:LEU:HD12	2.35	0.41
1:A:307:VAL:O	1:A:311:LEU:HD13	2.20	0.41
1:A:322:VAL:HG22	1:A:324:ILE:CD1	2.51	0.41
1:B:322:VAL:HG23	1:B:331:TRP:CD1	2.56	0.41
1:E:83:PHE:CE1	1:E:85:LEU:HG	2.51	0.41
1:F:140:VAL:O	1:F:147:LEU:HB2	2.21	0.41
1:F:311:LEU:CD1	1:F:320:HIS:CD2	2.94	0.41
1:B:281:THR:HG23	1:B:292:THR:HA	2.02	0.41
1:C:83:PHE:CE1	1:C:85:LEU:HG	2.53	0.41
1:C:126:PHE:CZ	1:C:182:ARG:HG3	2.55	0.41
1:D:67:PRO:HA	1:D:68:PRO:HD3	1.97	0.41
1:D:144:GLY:O	1:D:145:LYS:HD2	2.21	0.40
1:D:290:SER:HB3	1:E:157:LEU:HD21	2.03	0.40
1:A:8:ASN:HB3	1:A:15:PHE:HA	2.02	0.40
1:A:237:VAL:O	1:A:254:SER:HB3	2.22	0.40
1:B:207:ARG:CG	3:B:523:HOH:O	2.68	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ASN:HB2	1:C:340:VAL:O	2.21	0.40
1:C:300:LEU:HD23	1:C:300:LEU:HA	1.87	0.40
1:D:148:PRO:HB2	1:D:149:ALA:H	1.63	0.40
1:D:313:LEU:O	1:D:338:ASN:HA	2.21	0.40
1:E:311:LEU:CD1	1:E:320:HIS:CD2	2.95	0.40
1:F:264:LEU:HD11	1:F:282:VAL:CG2	2.51	0.40
1:A:87:ASP:OD1	1:A:87:ASP:C	2.64	0.40
1:A:205:LEU:HA	1:A:206:PRO:HD3	1.93	0.40
1:A:241:VAL:O	1:A:241:VAL:HG13	2.21	0.40
1:B:7:PHE:HA	1:B:22:LEU:HD12	2.03	0.40
1:A:149:ALA:O	1:A:151:LYS:HE3	2.21	0.40
1:B:241:VAL:HG21	1:B:284:TYR:CD1	2.56	0.40
1:A:24:VAL:HG13	1:A:33:VAL:HG22	2.03	0.40
1:C:173:LYS:HD2	1:E:287:ASP:OD1	2.22	0.40
1:C:218:ASP:OD1	1:F:225:LYS:HE2	2.22	0.40
1:E:317:SER:HB2	1:E:332:MET:HE1	2.03	0.40
1:F:250:HIS:CE1	1:F:344:TYR:HB3	2.57	0.40

All (2) 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:D:82:LYS:NZ	1:E:312:ASP:OD2[1_455]	1.87	0.33
3:A:509:HOH:O	3:B:520:HOH:O[4_555]	1.93	0.27

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	338/349 (97%)	317 (94%)	14 (4%)	7 (2%)	5 9
1	B	338/349 (97%)	319 (94%)	17 (5%)	2 (1%)	21 38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	338/349 (97%)	321 (95%)	14 (4%)	3 (1%)	14	27
1	D	338/349 (97%)	318 (94%)	17 (5%)	3 (1%)	14	27
1	E	338/349 (97%)	323 (96%)	13 (4%)	2 (1%)	21	38
1	F	338/349 (97%)	320 (95%)	16 (5%)	2 (1%)	21	38
All	All	2028/2094 (97%)	1918 (95%)	91 (4%)	19 (1%)	14	27

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLY
1	A	147	LEU
1	A	148	PRO
1	D	145	LYS
1	D	148	PRO
1	A	144	GLY
1	C	143	GLY
1	A	146	SER
1	A	142	THR
1	B	142	THR
1	B	143	GLY
1	C	36	GLY
1	D	147	LEU
1	E	144	GLY
1	F	288	PRO
1	E	288	PRO
1	F	36	GLY
1	A	288	PRO
1	C	288	PRO

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	298/304 (98%)	274 (92%)	24 (8%)	11	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	298/304 (98%)	272 (91%)	26 (9%)	9	21
1	C	298/304 (98%)	272 (91%)	26 (9%)	9	21
1	D	298/304 (98%)	272 (91%)	26 (9%)	9	21
1	E	298/304 (98%)	271 (91%)	27 (9%)	9	19
1	F	298/304 (98%)	274 (92%)	24 (8%)	11	23
All	All	1788/1824 (98%)	1635 (91%)	153 (9%)	10	21

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	47	THR
1	A	71	ILE
1	A	84	VAL
1	A	111	VAL
1	A	128	LEU
1	A	134	LEU
1	A	145	LYS
1	A	150	ILE
1	A	151	LYS
1	A	152	LEU
1	A	153	ASN
1	A	165	VAL
1	A	172	ILE
1	A	218	ASP
1	A	228	LEU
1	A	233	PHE
1	A	241	VAL
1	A	244	THR
1	A	252	LEU
1	A	300	LEU
1	A	311	LEU
1	A	322	VAL
1	A	342	THR
1	B	24	VAL
1	B	47	THR
1	B	71	ILE
1	B	84	VAL
1	B	111	VAL
1	B	128	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	134	LEU
1	B	141	LYS
1	B	142	THR
1	B	146	SER
1	B	147	LEU
1	B	151	LYS
1	B	152	LEU
1	B	153	ASN
1	B	165	VAL
1	B	172	ILE
1	B	218	ASP
1	B	228	LEU
1	B	233	PHE
1	B	241	VAL
1	B	244	THR
1	B	252	LEU
1	B	300	LEU
1	B	311	LEU
1	B	313	LEU
1	B	342	THR
1	C	24	VAL
1	C	47	THR
1	C	71	ILE
1	C	84	VAL
1	C	111	VAL
1	C	128	LEU
1	C	134	LEU
1	C	142	THR
1	C	146	SER
1	C	147	LEU
1	C	151	LYS
1	C	152	LEU
1	C	153	ASN
1	C	165	VAL
1	C	172	ILE
1	C	218	ASP
1	C	233	PHE
1	C	241	VAL
1	C	244	THR
1	C	252	LEU
1	C	285	LEU
1	C	300	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	311	LEU
1	C	313	LEU
1	C	322	VAL
1	C	342	THR
1	D	24	VAL
1	D	47	THR
1	D	71	ILE
1	D	84	VAL
1	D	111	VAL
1	D	128	LEU
1	D	134	LEU
1	D	141	LYS
1	D	146	SER
1	D	147	LEU
1	D	150	ILE
1	D	151	LYS
1	D	152	LEU
1	D	153	ASN
1	D	165	VAL
1	D	172	ILE
1	D	218	ASP
1	D	228	LEU
1	D	233	PHE
1	D	241	VAL
1	D	244	THR
1	D	252	LEU
1	D	300	LEU
1	D	311	LEU
1	D	322	VAL
1	D	342	THR
1	E	24	VAL
1	E	47	THR
1	E	71	ILE
1	E	84	VAL
1	E	111	VAL
1	E	128	LEU
1	E	134	LEU
1	E	141	LYS
1	E	142	THR
1	E	145	LYS
1	E	147	LEU
1	E	151	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	152	LEU
1	E	153	ASN
1	E	165	VAL
1	E	172	ILE
1	E	218	ASP
1	E	228	LEU
1	E	233	PHE
1	E	241	VAL
1	E	244	THR
1	E	252	LEU
1	E	300	LEU
1	E	311	LEU
1	E	313	LEU
1	E	340	VAL
1	E	342	THR
1	F	24	VAL
1	F	34	ARG
1	F	47	THR
1	F	71	ILE
1	F	84	VAL
1	F	111	VAL
1	F	128	LEU
1	F	134	LEU
1	F	141	LYS
1	F	145	LYS
1	F	147	LEU
1	F	151	LYS
1	F	152	LEU
1	F	153	ASN
1	F	165	VAL
1	F	172	ILE
1	F	218	ASP
1	F	233	PHE
1	F	241	VAL
1	F	244	THR
1	F	252	LEU
1	F	311	LEU
1	F	340	VAL
1	F	342	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	190	HIS
1	A	216	ASN
1	A	250	HIS
1	A	320	HIS
1	B	153	ASN
1	B	176	ASN
1	B	190	HIS
1	B	216	ASN
1	B	320	HIS
1	C	153	ASN
1	C	174	ASN
1	C	176	ASN
1	C	190	HIS
1	C	216	ASN
1	C	224	GLN
1	C	250	HIS
1	C	320	HIS
1	C	326	ASN
1	D	153	ASN
1	D	174	ASN
1	D	176	ASN
1	D	190	HIS
1	D	216	ASN
1	D	224	GLN
1	D	250	HIS
1	D	320	HIS
1	D	326	ASN
1	E	153	ASN
1	E	158	ASN
1	E	174	ASN
1	E	176	ASN
1	E	190	HIS
1	E	216	ASN
1	E	250	HIS
1	E	320	HIS
1	F	153	ASN
1	F	174	ASN
1	F	176	ASN
1	F	190	HIS
1	F	216	ASN
1	F	320	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](#)

6 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	PO4	B	401	-	4,4,4	1.05	0	6,6,6	1.72	3 (50%)
2	PO4	E	401	-	4,4,4	0.84	0	6,6,6	1.01	0
2	PO4	F	401	-	4,4,4	1.94	1 (25%)	6,6,6	1.20	1 (16%)
2	PO4	A	401	-	4,4,4	0.98	0	6,6,6	1.01	0
2	PO4	D	401	-	4,4,4	1.36	0	6,6,6	1.18	1 (16%)
2	PO4	C	401	-	4,4,4	1.46	1 (25%)	6,6,6	1.29	1 (16%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	PO4	P-O1	3.69	1.59	1.50
2	C	401	PO4	P-O1	2.81	1.57	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	PO4	O3-P-O1	-2.70	101.40	110.95
2	B	401	PO4	O3-P-O2	2.33	115.15	107.91
2	C	401	PO4	O4-P-O2	-2.27	100.86	107.91
2	D	401	PO4	O4-P-O2	2.14	114.56	107.91
2	F	401	PO4	O3-P-O2	-2.10	101.38	107.91
2	B	401	PO4	O4-P-O1	2.00	118.04	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PO4	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	342/349 (97%)	0.86	45 (13%) 7 6	30, 46, 82, 102	0
1	B	342/349 (97%)	0.89	35 (10%) 12 10	28, 48, 84, 130	0
1	C	342/349 (97%)	0.64	24 (7%) 22 20	28, 43, 80, 101	0
1	D	342/349 (97%)	0.77	29 (8%) 16 14	27, 44, 79, 113	0
1	E	342/349 (97%)	0.71	29 (8%) 16 14	28, 45, 80, 112	0
1	F	342/349 (97%)	0.55	20 (5%) 29 25	28, 45, 81, 109	0
All	All	2052/2094 (97%)	0.74	182 (8%) 15 13	27, 45, 81, 130	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	146	SER	7.0
1	C	172	ILE	6.8
1	D	142	THR	5.8
1	D	139	ALA	5.6
1	E	172	ILE	5.4
1	A	171	ASN	5.4
1	A	144	GLY	5.1
1	B	228	LEU	4.9
1	A	172	ILE	4.8
1	A	147	LEU	4.5
1	D	144	GLY	4.5
1	C	171	ASN	4.3
1	A	143	GLY	4.3
1	E	171	ASN	4.3
1	E	231	PHE	4.2
1	E	309	LYS	4.1
1	B	172	ILE	4.1
1	B	316	VAL	4.1
1	A	150	ILE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	218	ASP	4.0
1	B	171	ASN	3.9
1	B	334	TRP	3.9
1	B	307	VAL	3.9
1	D	149	ALA	3.8
1	D	141	LYS	3.8
1	E	313	LEU	3.8
1	F	143	GLY	3.7
1	B	338	ASN	3.6
1	D	320	HIS	3.6
1	D	172	ILE	3.6
1	F	316	VAL	3.5
1	D	171	ASN	3.4
1	F	171	ASN	3.4
1	A	140	VAL	3.4
1	B	144	GLY	3.4
1	B	339	ALA	3.4
1	F	172	ILE	3.4
1	C	315	VAL	3.4
1	E	315	VAL	3.4
1	A	316	VAL	3.4
1	A	146	SER	3.3
1	D	140	VAL	3.3
1	B	186	LYS	3.3
1	C	107	PHE	3.3
1	A	314	THR	3.2
1	C	143	GLY	3.2
1	F	144	GLY	3.2
1	A	145	LYS	3.2
1	F	346	GLN	3.2
1	D	145	LYS	3.2
1	C	144	GLY	3.2
1	E	314	THR	3.2
1	C	346	GLN	3.2
1	A	179	VAL	3.2
1	A	165	VAL	3.1
1	C	186	LYS	3.1
1	A	142	THR	3.1
1	C	123	TYR	3.0
1	E	142	THR	3.0
1	C	189	ASP	3.0
1	C	36	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	311	LEU	3.0
1	B	120	GLN	3.0
1	D	150	ILE	3.0
1	E	71	ILE	3.0
1	D	334	TRP	3.0
1	A	315	VAL	2.9
1	D	120	GLN	2.9
1	B	227	GLY	2.9
1	A	335	CYS	2.9
1	B	345	PRO	2.9
1	E	108	ALA	2.9
1	A	218	ASP	2.9
1	C	312	ASP	2.9
1	E	189	ASP	2.9
1	E	317	SER	2.9
1	B	315	VAL	2.9
1	C	109	GLU	2.9
1	A	312	ASP	2.8
1	B	236	VAL	2.8
1	A	149	ALA	2.8
1	F	321	GLU	2.8
1	B	140	VAL	2.8
1	F	142	THR	2.8
1	E	316	VAL	2.7
1	A	346	GLN	2.7
1	E	230	ASP	2.7
1	D	338	ASN	2.7
1	E	343	PHE	2.7
1	B	231	PHE	2.6
1	E	338	ASN	2.6
1	C	0	SER	2.6
1	D	317	SER	2.6
1	A	336	LYS	2.6
1	D	108	ALA	2.6
1	E	186	LYS	2.6
1	B	230	ASP	2.6
1	B	223	ILE	2.6
1	B	128	LEU	2.6
1	A	0	SER	2.6
1	B	341	ALA	2.6
1	D	124	GLU	2.5
1	C	316	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	344	TYR	2.5
1	A	189	ASP	2.5
1	A	344	TYR	2.4
1	E	312	ASP	2.4
1	F	311	LEU	2.4
1	F	146	SER	2.4
1	E	339	ALA	2.4
1	D	318	LYS	2.4
1	A	313	LEU	2.4
1	A	236	VAL	2.4
1	D	186	LYS	2.4
1	D	29	ASP	2.4
1	A	190	HIS	2.4
1	A	188	VAL	2.4
1	F	339	ALA	2.4
1	B	333	LEU	2.3
1	F	315	VAL	2.3
1	A	128	LEU	2.3
1	D	233	PHE	2.3
1	C	111	VAL	2.3
1	A	174	ASN	2.3
1	A	148	PRO	2.3
1	A	311	LEU	2.3
1	A	332	MET	2.3
1	E	320	HIS	2.3
1	C	128	LEU	2.3
1	F	186	LYS	2.3
1	B	319	VAL	2.3
1	F	165	VAL	2.3
1	B	226	TYR	2.3
1	B	142	THR	2.2
1	F	244	THR	2.2
1	C	220	GLY	2.2
1	B	165	VAL	2.2
1	D	315	VAL	2.2
1	A	139	ALA	2.2
1	E	145	LYS	2.2
1	C	165	VAL	2.2
1	E	187	PRO	2.2
1	C	187	PRO	2.2
1	D	165	VAL	2.2
1	D	319	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	344	TYR	2.2
1	A	187	PRO	2.2
1	A	194	PHE	2.2
1	E	183	LYS	2.2
1	B	311	LEU	2.1
1	B	342	THR	2.1
1	D	143	GLY	2.1
1	C	219	ILE	2.1
1	E	123	TYR	2.1
1	A	186	LYS	2.1
1	A	334	TRP	2.1
1	A	244	THR	2.1
1	D	147	LEU	2.1
1	F	313	LEU	2.1
1	E	310	SER	2.1
1	B	111	VAL	2.1
1	B	346	GLN	2.1
1	B	139	ALA	2.1
1	F	128	LEU	2.1
1	A	195	TYR	2.1
1	F	317	SER	2.1
1	B	147	LEU	2.1
1	C	338	ASN	2.1
1	A	321	GLU	2.1
1	B	332	MET	2.1
1	A	320	HIS	2.1
1	F	190	HIS	2.1
1	E	346	GLN	2.0
1	A	107	PHE	2.0
1	D	135	PHE	2.0
1	B	134	LEU	2.0
1	F	192	ASP	2.0
1	A	120	GLN	2.0
1	C	188	VAL	2.0
1	E	319	VAL	2.0
1	B	309	LYS	2.0
1	A	123	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	PO4	F	401	5/5	0.73	0.12	45,47,57,87	0
2	PO4	E	401	5/5	0.75	0.12	51,65,75,85	0
2	PO4	B	401	5/5	0.76	0.12	56,57,72,107	0
2	PO4	A	401	5/5	0.78	0.14	60,63,80,99	0
2	PO4	C	401	5/5	0.85	0.09	42,45,63,86	0
2	PO4	D	401	5/5	0.87	0.10	39,39,63,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.