



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:34 PM GMT

PDB ID : 4S1T
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

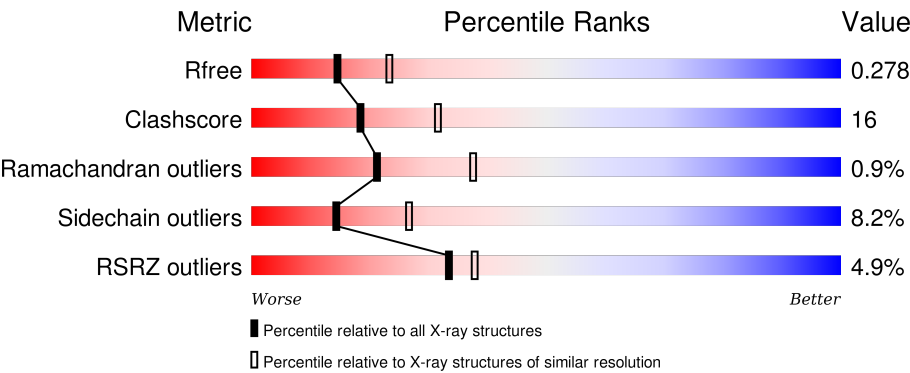
1 Overall quality at a glance i

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	349	
1	B	349	
1	C	349	
1	D	349	
1	E	349	

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Mol	Chain	Length	Quality of chain
1	F	349	<div><div><div>%</div><div><div></div></div><div>74%</div><div>19%</div><div><div></div><div></div></div></div></div>

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:

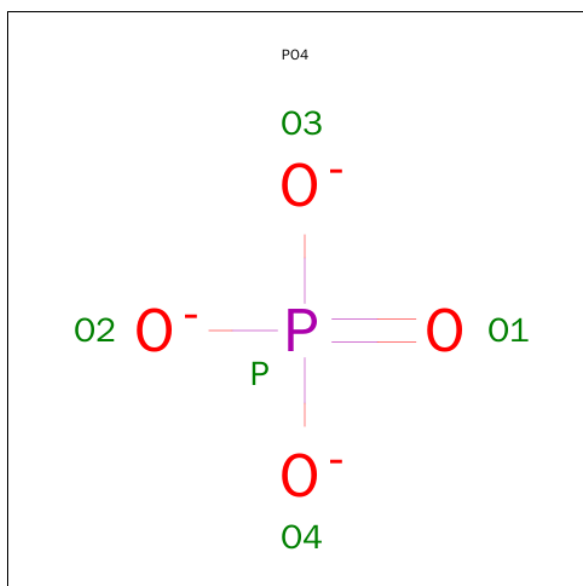
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P0C6X1
A	26	ALA	ILE	ENGINEERED MUTATION	UNP P0C6X1
A	52	ALA	ASN	ENGINEERED MUTATION	UNP P0C6X1
B	0	SER	-	EXPRESSION TAG	UNP P0C6X1
B	26	ALA	ILE	ENGINEERED MUTATION	UNP P0C6X1
B	52	ALA	ASN	ENGINEERED MUTATION	UNP P0C6X1
C	0	SER	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	52	ALA	ASN	ENGINEERED MUTATION	UNP P0C6X1

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is water.

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

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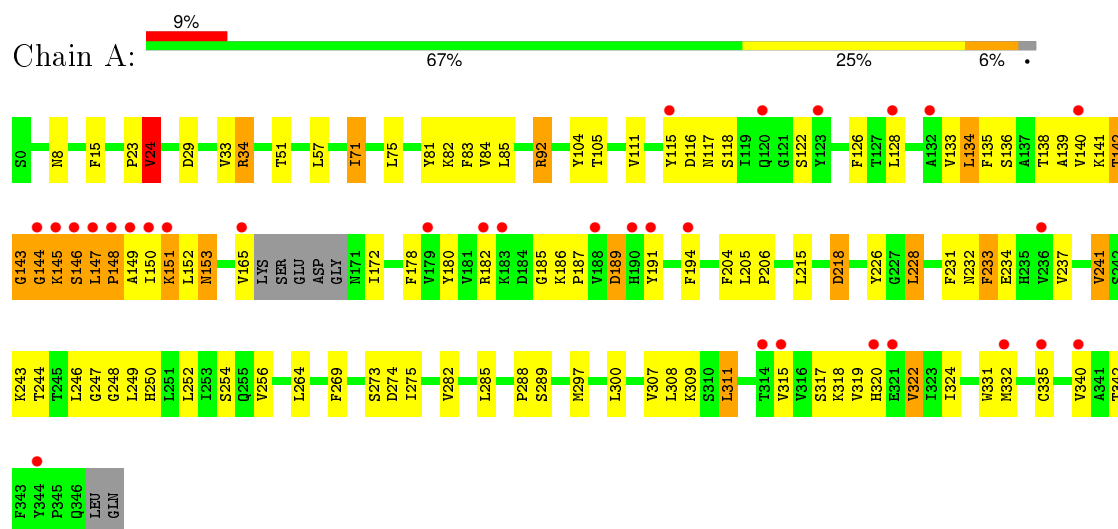
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	109	Total 109	O 109	0	0
3	E	102	Total 102	O 102	0	0
3	F	94	Total 94	O 94	0	0

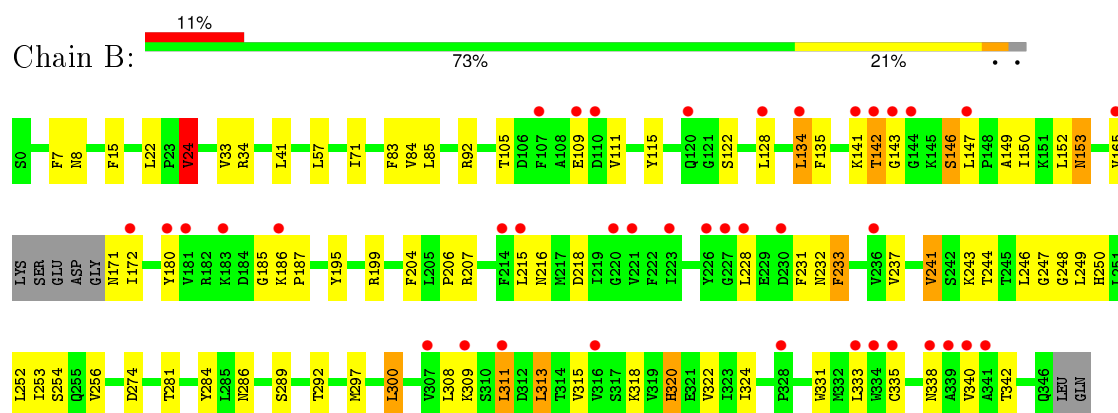
3 Residue-property plots

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

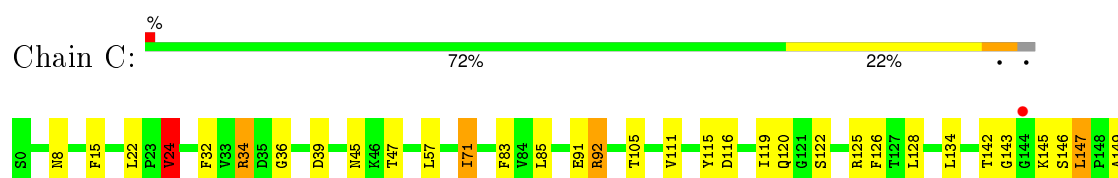
• Molecule 1: Uridylate-specific endoribonuclease

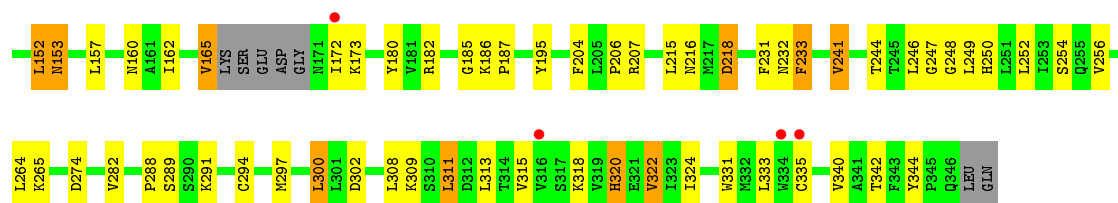


• Molecule 1: Uridylate-specific endoribonuclease

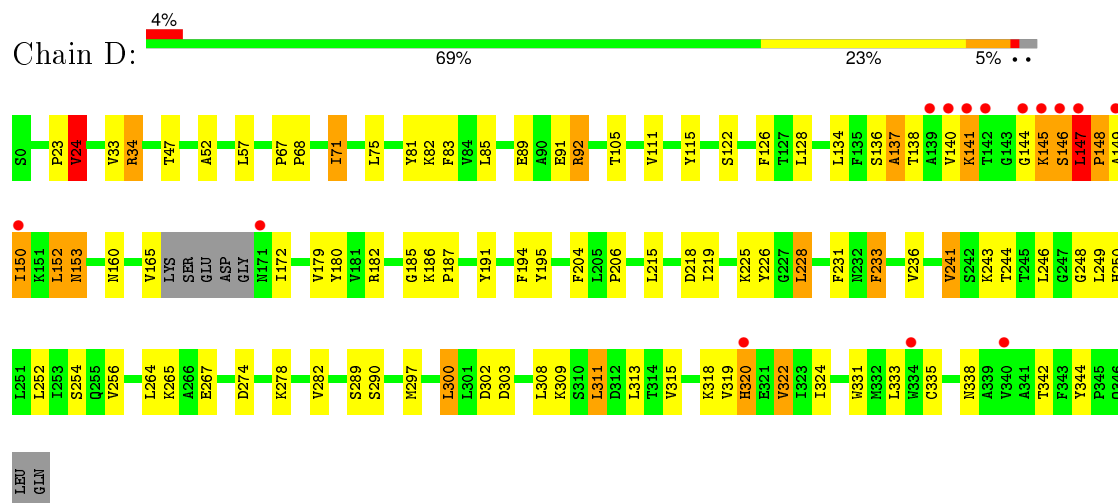


• Molecule 1: Uridylate-specific endoribonuclease

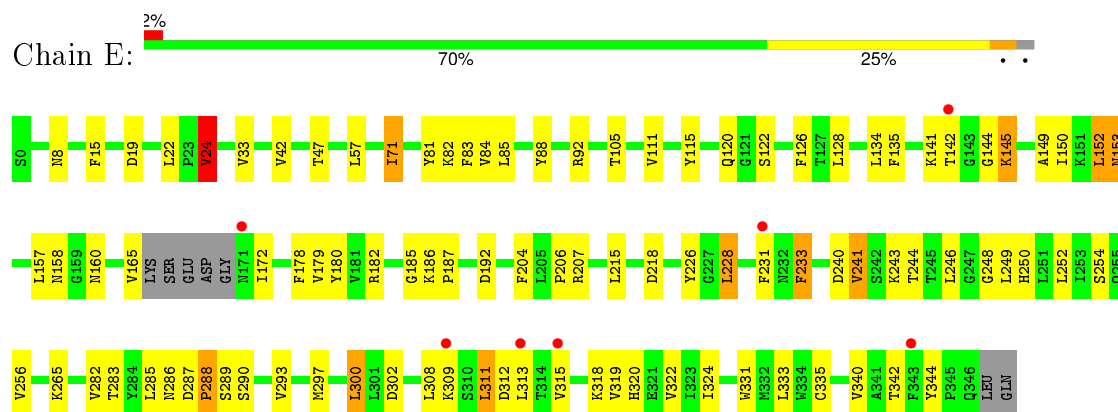




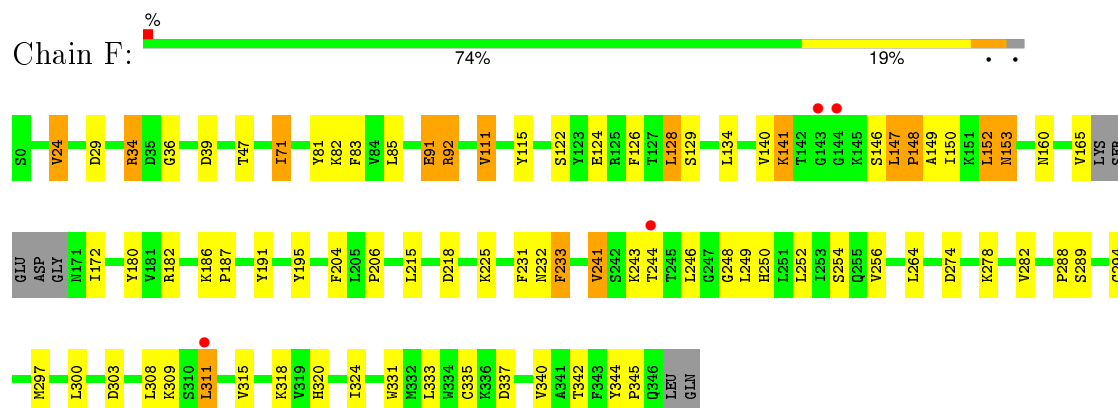
• Molecule 1: Uridylate-specific endoribonuclease



• Molecule 1: Uridylate-specific endoribonuclease



• Molecule 1: Uridylate-specific endoribonuclease



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 49.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (43.22-2.50) 96.3 (49.95-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.241 , 0.285 0.236 , 0.278	Depositor DCC
R_{free} test set	4357 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 89289 reflections	Xtriage
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

Xtriage'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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.87	0/2737	0.77	2/3716 (0.1%)
1	B	0.88	0/2737	0.75	1/3716 (0.0%)
1	C	0.80	0/2737	0.79	5/3716 (0.1%)
1	D	0.79	0/2737	0.79	5/3716 (0.1%)
1	E	0.81	1/2737 (0.0%)	0.79	3/3716 (0.1%)
1	F	0.78	0/2737	0.77	4/3716 (0.1%)
All	All	0.82	1/16422 (0.0%)	0.78	20/22296 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	3
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	88	TYR	CD2-CE2	5.41	1.47	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	ALA	C-N-CA	10.82	148.75	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92	ARG	NE-CZ-NH1	-7.87	116.37	120.30
1	D	137	ALA	O-C-N	-7.29	111.03	122.70
1	E	24	VAL	CB-CA-C	-6.85	98.39	111.40
1	F	92	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	C	24	VAL	CB-CA-C	-6.72	98.63	111.40
1	E	92	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	F	24	VAL	CB-CA-C	-6.28	99.47	111.40
1	C	92	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	B	24	VAL	CB-CA-C	-6.14	99.74	111.40
1	F	92	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	D	24	VAL	CB-CA-C	-5.76	100.46	111.40
1	A	92	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	24	VAL	CB-CA-C	-5.67	100.64	111.40
1	D	92	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	C	92	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	C	116	ASP	CB-CG-OD1	5.26	123.03	118.30
1	F	300	LEU	CB-CG-CD2	5.22	119.88	111.00
1	E	207	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	C	207	ARG	NE-CZ-NH2	-5.08	117.76	120.30

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 ⓘ

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	132	0
1	B	2679	0	2667	61	0
1	C	2679	0	2667	70	0
1	D	2679	0	2667	109	1
1	E	2679	0	2667	75	1
1	F	2679	0	2667	70	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	15	1
3	B	49	0	0	15	1
3	C	102	0	0	7	0
3	D	109	0	0	7	0
3	E	102	0	0	7	0
3	F	94	0	0	15	0
All	All	16623	0	16001	499	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 (499) 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	1.43
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	1.19
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:D:149:ALA:HB2	1:D:180:TYR:CE1	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:149:ALA:HB2	1:E:180:TYR:CE1	1.96	1.00
1:A:143:GLY:C	1:A:145:LYS:CB	2.30	0.99
1:A:146:SER:O	1:A:147:LEU:HB2	1.59	0.99
1:A:297:MET:HE1	1:A:324:ILE:HG21	1.44	0.99
1:A:142:THR:C	1:A:145:LYS:CB	2.30	0.99
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:318:LYS:NZ	3:A:540:HOH:O	1.98	0.94
1:A:145:LYS:HD3	1:A:145:LYS:O	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:141:LYS:HD2	1:D:141:LYS:C	1.84	0.94
1:D:150:ILE:CG2	1:D:195:TYR:OH	2.15	0.93
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:140:VAL:O	1:A:146:SER:O	1.91	0.89
1:A:117:ASN:HB3	1:A:136:SER:HB2	1.52	0.89
1:E:297:MET:HE1	1:E:324:ILE:HG21	1.53	0.88
1:D:297:MET:HE3	1:D:324:ILE:HG21	1.54	0.88
1:D:140:VAL:HG12	1:D:180:TYR:OH	1.74	0.88
1:D:141:LYS:CD	1:D:141:LYS:C	2.41	0.87
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:C:297:MET:HE1	1:C:324:ILE:HG21	1.58	0.84
1:F:297:MET:HE1	1:F:324:ILE:HG21	1.59	0.84
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:140:VAL:O	1:A:146:SER:HA	1.78	0.82
1:B:297:MET:HE1	1:B:324:ILE:HG21	1.60	0.82
1:A:142:THR:O	1:A:145:LYS:HB2	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:231:PHE:HA	1:E:340:VAL:HG13	1.63	0.79
1:A:145:LYS:CD	1:A:145:LYS:O	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:143:GLY:N	1:A:145:LYS:CB	2.48	0.76
1:A:144:GLY:N	1:A:145:LYS:CB	2.47	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:O	1:D:141:LYS:HD2	1.86	0.74
1:C:297:MET:CE	1:C:324:ILE:HG21	2.18	0.73
1:A:133:VAL:O	3:A:506:HOH:O	2.06	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:A:141:LYS:C	1:A:142:THR:HG23	2.13	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: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:A:141:LYS:C	1:A:142:THR:CG2	2.61	0.68
1:E:158:ASN:O	3:E:507:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:N	3:A:506:HOH:O	2.23	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:E:149:ALA:CB	1:E:180:TYR:CE1	2.78	0.65
1:D:92:ARG:NH2	3:D:575:HOH:O	2.28	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:318:LYS:HD2	1:C:320:HIS:CE1	2.32	0.65
1:C:45:ASN:O	3:C:519:HOH:O	2.14	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:HD22	1:E:153:ASN:H	1.44	0.64
1:A:297:MET:HE1	1:A:324:ILE:CG2	2.24	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: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:A:147:LEU:O	1:A:148:PRO:C	2.37	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:H	1:F:153:ASN:HD22	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

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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:D:150:ILE:HG21	1:D:195:TYR:HH	1.65	0.61
1:B:318:LYS:HD2	1:B:320:HIS:CE1	2.35	0.61
1:B:204:PHE:CG	1:B:256:VAL:HG21	2.34	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: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:219:ILE:HG13	3:D:605:HOH:O	2.01	0.60
1:D:153:ASN:H	1:D:153:ASN:HD22	1.49	0.60
1:D:322:VAL:HG13	1:D:331:TRP:CD1	2.36	0.60
1:D:308:LEU:HA	1:D:311:LEU:HD22	1.83	0.60
1:A:186:LYS:NZ	3:A:535:HOH:O	2.11	0.60
1:D:146:SER:O	1:D:147:LEU:C	2.39	0.60
1:D:144:GLY:O	1:D:145:LYS:CG	2.49	0.60
1:D:52:ALA:O	3:D:502:HOH:O	2.17	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:H	1:A:153:ASN:HD22	1.51	0.59
1:A:141:LYS:O	1:A:142:THR:HG23	2.01	0.59
1:E:308:LEU:HA	1:E:311:LEU:HD22	1.85	0.59
1:C:153:ASN:HD22	1:C:153:ASN:H	1.50	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:311:LEU:CD1	1:C:320:HIS:HD2	2.15	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:E:150:ILE:HB	1:E:179:VAL:HB	1.86	0.58
1:C:83:PHE:HE1	1:C:85:LEU:HG	1.67	0.58
1:C:160:ASN:OD1	1:E:265:LYS:HG3	2.03	0.58
1:D:136:SER:OG	1:D:138:THR:HG22	2.04	0.58
1:B:115:TYR:HB3	1:B:122:SER:HB3	1.86	0.58
1:A:249:LEU:HD12	1:A:254:SER:HB3	1.85	0.57
1:D:204:PHE:CG	1:D:256:VAL:HG21	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:LYS:HG3	1:F:187:PRO:HD2	1.84	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:311:LEU:CD1	1:D:320:HIS:HD2	2.18	0.56
1:A:332:MET:HE3	3:A:534:HOH:O	2.05	0.56
1:D:89:GLU:O	3:D:513:HOH:O	2.17	0.56
1:A:143:GLY:O	1:A:144:GLY:C	2.44	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:F:297:MET:CE	1:F:324:ILE:HD13	2.36	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:E:57:LEU:HD11	1:E:105:THR:HG21	1.86	0.56
1:A:142:THR:H	1:A:145:LYS:CB	2.19	0.55
1:D:140:VAL:O	1:D:141:LYS:HB3	2.07	0.55
1:A:311:LEU:CD1	1:A:320:HIS:HD2	2.19	0.55
1:A:104:TYR:HB2	3:A:509:HOH:O	2.07	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: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:F:231:PHE:O	1:F:233:PHE:N	2.40	0.54
1:D:231:PHE:O	1:D:233:PHE:N	2.39	0.54
1:B:186:LYS:HG3	1:B:187:PRO:HD2	1.90	0.54
1:A:83:PHE:HE1	1:A:85:LEU:HG	1.72	0.54
1:D:322:VAL:CG1	1:D:331:TRP:CD1	2.92	0.53
1:E:311:LEU:HD12	1:E:320:HIS:HD2	1.73	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:C:241:VAL:O	1:C:241:VAL:HG13	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:140:VAL:O	1:A:146:SER:C	2.47	0.53
1:B:311:LEU:O	3:B:527:HOH:O	2.19	0.53
1:B:311:LEU:HD12	1:B:320:HIS:CD2	2.43	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:297:MET:HE1	1:F:324:ILE:CG2	2.35	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:A:142:THR:N	1:A:145:LYS:HB2	2.24	0.52
1:F:315:VAL:O	1:F:335:CYS:HB2	2.09	0.52
1:D:141:LYS:HD2	1:D:141:LYS:N	2.22	0.52
1:D:297:MET:HE3	1:D:324:ILE:CG2	2.34	0.52
1:C:315:VAL:O	1:C:335:CYS:HB2	2.09	0.52
1:F:83:PHE:HE1	1:F:85:LEU:HG	1.75	0.52
1:F:150:ILE:HG12	1:F:191:TYR:CG	2.45	0.52
1:C:157:LEU:HG	1:E:283:THR:HG23	1.92	0.52
1:A:138:THR:HG22	1:A:139:ALA:N	2.25	0.52
1:D:311:LEU:HD12	1:D:320:HIS:HD2	1.74	0.52
1:C:160:ASN:HB3	1:E:285:LEU:HD11	1.90	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:A:126:PHE:CZ	1:A:182:ARG:HG3	2.45	0.52
1:B:109:GLU:HB2	3:B:525:HOH:O	2.09	0.51
1:D:241:VAL:HG13	1:D:241:VAL:O	2.10	0.51
1:E:297:MET:HE1	1:E:324:ILE:CG2	2.33	0.51
1:F:241:VAL:HG13	1:F:241:VAL:O	2.10	0.51
1:D:231:PHE:CZ	1:D:309:LYS:HG2	2.45	0.51
1:D:246:LEU:HB2	1:D:289:SER:OG	2.11	0.51
1:B:231:PHE:CZ	1:B:309:LYS:HG2	2.46	0.51
1:D:92:ARG:NH1	1:D:274:ASP:OD2	2.32	0.51
1:D:144:GLY:C	1:D:145:LYS:HG2	2.30	0.51
1:F:186:LYS:NZ	3:F:559:HOH:O	2.39	0.51
1:A:231:PHE:CZ	1:A:309:LYS:HG2	2.46	0.51
1:E:248:GLY:C	1:E:250:HIS:HD2	2.15	0.51
1:B:149:ALA:HB2	1:B:180:TYR:CZ	2.44	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:153:ASN:N	1:E:153:ASN:HD22	2.06	0.50
1:D:71:ILE:CD1	1:D:152:LEU:HD21	2.42	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:F:248:GLY:C	1:F:250:HIS:HD2	2.15	0.49
1:F:126:PHE:CZ	1:F:182:ARG:HG3	2.47	0.49
1:B:153:ASN:HD22	1:B:153:ASN:N	2.10	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:C:322:VAL:HG22	1:C:324:ILE:HD11	1.95	0.49
1:A:151:LYS:H	1:A:151:LYS:HE3	1.78	0.48
1:C:265:LYS:HG3	1:D:160:ASN:OD1	2.12	0.48
1:B:216:ASN:HD22	1:B:216:ASN:N	2.09	0.48
1:F:141:LYS:HE2	1:F:146:SER:HB3	1.96	0.48
1:F:92:ARG:NH1	1:F:274:ASP:OD2	2.42	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:F:182:ARG:NE	3:F:550:HOH:O	2.46	0.48
1:E:231:PHE:CE2	1:E:309:LYS:HG2	2.48	0.48
1:F:231:PHE:CZ	1:F:309:LYS:HG2	2.49	0.48
1:B:187:PRO:HB3	3:B:536:HOH:O	2.12	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:297:MET:CE	1:D:324:ILE:HD13	2.44	0.47
1:E:318:LYS:HD2	1:E:320:HIS:HE1	1.72	0.47
1:D:250:HIS:CE1	1:D:344:TYR:CB	2.97	0.47
1:C:311:LEU:CD1	1:C:320:HIS:CD2	2.96	0.47
1:D:250:HIS:CE1	1:D:344:TYR:HB2	2.49	0.47
1:E:206:PRO:HG3	1:E:215:LEU:HD12	1.96	0.47
1:C:204:PHE:CG	1:C:256:VAL:HG21	2.49	0.47
1:C:24:VAL:HA	1:C:32:PHE:O	2.13	0.47
1:B:231:PHE:CE2	1:B:309:LYS:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:VAL:O	3:E:597:HOH:O	2.20	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:23:PRO:HB2	1:A:34:ARG:HB2	1.96	0.47
1:A:148:PRO:CG	1:A:189:ASP:O	2.63	0.47
1:C:153:ASN:HD22	1:C:153:ASN:N	2.10	0.47
1:B:253:ILE:N	3:B:506:HOH:O	2.12	0.47
1:E:250:HIS:CE1	1:E:344:TYR:CB	2.98	0.47
1:B:134:LEU:HD22	1:B:135:PHE:N	2.30	0.47
1:A:92:ARG:NH1	1:A:274:ASP:OD2	2.44	0.47
1:B:313:LEU:CD1	3:B:527:HOH:O	2.45	0.47
1:B:57:LEU:HD11	1:B:105:THR:HG21	1.97	0.47
1:E:135:PHE:HA	1:E:178:PHE:O	2.15	0.46
1:F:81:TYR:CE2	1:F:82:LYS:HG3	2.50	0.46
1:F:29:ASP:HB3	3:F:574:HOH:O	2.15	0.46
1:F:147:LEU:HD22	1:F:148:PRO:HD2	1.97	0.46
1:E:246:LEU:HB2	1:E:289:SER:OG	2.14	0.46
1:E:71:ILE:CD1	1:E:152:LEU:HD21	2.46	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:C:311:LEU:HG	1:C:333:LEU:HD22	1.97	0.46
1:E:81:TYR:OH	1:E:82:LYS:HE3	2.15	0.46
1:C:232:ASN:H	1:C:340:VAL:HB	1.79	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:C:247:GLY:HA2	3:C:504:HOH:O	2.15	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:E:250:HIS:CE1	1:E:344:TYR:HB2	2.51	0.46
1:B:300:LEU:HA	1:B:300:LEU:HD23	1.83	0.46
1:F:150:ILE:HG23	1:F:195:TYR:CZ	2.51	0.45
1:C:248:GLY:C	1:C:250:HIS:HD2	2.20	0.45
1:A:151:LYS:HG3	1:A:178:PHE:CE1	2.52	0.45
1:D:140:VAL:HG13	1:D:180:TYR:CZ	2.42	0.45
1:D:248:GLY:C	1:D:250:HIS:HD2	2.20	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:F:146:SER:O	1:F:147:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:HG23	1:B:195:TYR:CZ	2.51	0.45
1:B:311:LEU:C	3:B:527:HOH:O	2.53	0.45
1:E:126:PHE:CZ	1:E:182:ARG:HG3	2.52	0.45
1:D:264:LEU:HD11	1:D:282:VAL:CG2	2.46	0.45
1:D:185:GLY:O	1:D:186:LYS:HD2	2.17	0.45
1:B:206:PRO:HG3	1:B:215:LEU:HD12	1.99	0.45
1:A:232:ASN:H	1:A:340:VAL:HB	1.82	0.45
1:D:206:PRO:HG3	1:D:215:LEU:HD12	1.99	0.45
1:D:231:PHE:CE2	1:D:309:LYS:HG2	2.51	0.45
1:E:231:PHE:O	1:E:233:PHE:N	2.47	0.44
1:F:318:LYS:HD2	1:F:320:HIS:HE1	1.81	0.44
1:E:226:TYR:O	1:E:228:LEU:HD13	2.17	0.44
1:E:300:LEU:HD23	1:E:300:LEU:HA	1.78	0.44
1:F:331:TRP:CZ3	1:F:345:PRO:HD3	2.52	0.44
1:F:231:PHE:HA	1:F:340:VAL:CG1	2.33	0.44
1:C:231:PHE:CZ	1:C:309:LYS:HG2	2.52	0.44
1:D:318:LYS:HD2	1:D:320:HIS:ND1	2.32	0.44
1:B:185:GLY:O	1:B:186:LYS:HD2	2.17	0.44
1:A:206:PRO:HG3	1:A:215:LEU:HD12	1.99	0.44
1:E:22:LEU:O	1:E:24:VAL:HG22	2.16	0.44
1:D:278:LYS:NZ	3:D:512:HOH:O	2.27	0.44
1:D:23:PRO:HB2	1:D:34:ARG:HB2	2.00	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:150:ILE:HG22	1:D:195:TYR:OH	2.09	0.44
1:A:322:VAL:HG22	1:A:324:ILE:HD11	2.00	0.44
1:A:311:LEU:HD12	1:A:320:HIS:HD2	1.82	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:F:294:CYS:HA	3:F:506:HOH:O	2.18	0.44
1:F:71:ILE:CD1	1:F:152:LEU:HD21	2.48	0.44
1:A:204:PHE:CG	1:A:256:VAL:HG21	2.53	0.44
1:A:147:LEU:O	1:A:180:TYR:CE1	2.71	0.44
1:B:253:ILE:CB	3:B:506:HOH:O	2.63	0.44
1:E:243:LYS:HB2	1:E:243:LYS:HE2	1.86	0.44
1:D:249:LEU:CD1	1:D:254:SER:HB3	2.46	0.43
1:C:92:ARG:NH2	3:C:600:HOH:O	2.51	0.43
1:E:322:VAL:HG23	1:E:331:TRP:CD1	2.53	0.43
1:D:243:LYS:HB2	1:D:243:LYS:HE2	1.84	0.43
1:B:232:ASN:HB2	1:B:340:VAL:O	2.18	0.43
1:B:297:MET:HE1	1:B:324:ILE:CG2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:SER:CB	3:A:534:HOH:O	2.65	0.43
1:A:234:GLU:HB2	3:A:550:HOH:O	2.18	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:D:150:ILE:HG23	1:D:191:TYR:HB3	2.00	0.43
1:C:297:MET:HE1	1:C:324:ILE:HD13	2.00	0.43
1:C:22:LEU:O	1:C:24:VAL:HG22	2.18	0.43
1:A:243:LYS:HE2	1:A:243:LYS:HB2	1.79	0.43
1:D:81:TYR:CE2	1:D:82:LYS:HG3	2.53	0.43
1:B:237:VAL:O	1:B:254:SER:HB3	2.19	0.43
1:C:250:HIS:CE1	1:C:344:TYR:HB2	2.54	0.43
1:F:250:HIS:CE1	1:F:344:TYR:CB	3.01	0.43
1:F:243:LYS:HE2	1:F:243:LYS:HB2	1.81	0.43
1:E:250:HIS:CE1	1:E:344:TYR:HB3	2.54	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:F:160:ASN:OD1	3:F:591:HOH:O	2.21	0.43
1:F:250:HIS:CE1	1:F:344:TYR:HB2	2.54	0.43
1:C:206:PRO:HG3	1:C:215:LEU:HD12	2.01	0.43
1:B:8:ASN:HB3	1:B:15:PHE:HA	2.00	0.43
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: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: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:B:311:LEU:CD1	1:B:320:HIS:CD2	2.99	0.42
1:F:182:ARG:HD3	3:F:550:HOH:O	2.20	0.42
1:E:318:LYS:HG2	1:E:319:VAL:N	2.35	0.42
1:B:243:LYS:HE2	1:B:243:LYS:HB2	1.85	0.42
1:D:300:LEU:HA	1:D:300:LEU:HD23	1.93	0.42
1:C:8:ASN:HB3	1:C:15:PHE:HA	2.02	0.42
1:C:250:HIS:CE1	1:C:344:TYR:CB	3.02	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:VAL:HG21	1:E:286:ASN:O	2.19	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:D:140:VAL:HG11	1:D:180:TYR:CD2	2.53	0.42
1:E:248:GLY:C	1:E:250:HIS:CD2	2.93	0.42
1:A:226:TYR:O	1:A:228:LEU:HD13	2.20	0.42
1:F:34:ARG:HD3	1:F:39:ASP:OD1	2.19	0.42
1:F:231:PHE:CE2	1:F:309:LYS:HG2	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:A:81:TYR:CE2	1:A:82:LYS:HG3	2.55	0.42
1:A:232:ASN:HB2	1:A:340:VAL:O	2.19	0.41
1:D:236:VAL:HG22	3:D:581:HOH:O	2.19	0.41
1:A:29:ASP:HA	1:A:51:THR:OG1	2.21	0.41
1:D:265:LYS:HG3	1:E:160:ASN:OD1	2.20	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:C:185:GLY:O	1:C:186:LYS:HD2	2.21	0.41
1:C:248:GLY:C	1:C:250:HIS:CD2	2.94	0.41
1:A:318:LYS:HE3	1:A:320:HIS:HE1	1.85	0.41
1:D:318:LYS:HG2	1:D:319:VAL:N	2.36	0.41
1:C:71:ILE:CD1	1:C:152:LEU:HD21	2.51	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:C:173:LYS:NZ	1:E:287:ASP:OD1	2.53	0.41
1:B:241:VAL:HG13	1:B:241:VAL:O	2.20	0.41
1:B:215:LEU:C	1:B:216:ASN:HD22	2.24	0.41
1:C:119:ILE:O	1:C:120:GLN:C	2.59	0.41
1:A:311:LEU:HD12	1:A:320:HIS:CD2	2.56	0.41
1:F:129:SER:HB2	3:F:550:HOH:O	2.19	0.41
1:C:248:GLY:HA2	3:C:591:HOH:O	2.20	0.41
1:B:248:GLY:C	1:B:250:HIS:CD2	2.94	0.41
1:C:291:LYS:HD3	1:C:294:CYS:HA	2.02	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:A:322:VAL:HG22	1:A:324:ILE:CD1	2.51	0.41
1:A:307:VAL:O	1:A:311:LEU:HD13	2.20	0.41
1:F:311:LEU:CD1	1:F:320:HIS:CD2	2.94	0.41
1:A:246:LEU:HD12	1:A:247:GLY:N	2.36	0.41
1:E:241:VAL:O	1:E:241:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:285:LEU:N	1:A:285:LEU:HD12	2.35	0.41
1:B:322:VAL:HG23	1:B:331:TRP:CD1	2.56	0.41
1:E:297:MET:CE	1:E:324:ILE:HD13	2.51	0.41
1:C:83:PHE:CE1	1:C:85:LEU:HG	2.53	0.41
1:C:215:LEU:C	1:C:216:ASN:HD22	2.24	0.41
1:C:126:PHE:CZ	1:C:182:ARG:HG3	2.55	0.41
1:B:281:THR:HG23	1:B:292:THR:HA	2.02	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:D:148:PRO:HB2	1:D:149:ALA:H	1.63	0.40
1:E:311:LEU:CD1	1:E:320:HIS:CD2	2.95	0.40
1:A:237:VAL:O	1:A:254:SER:HB3	2.22	0.40
1:C:232:ASN:HB2	1:C:340:VAL:O	2.21	0.40
1:F:264:LEU:HD11	1:F:282:VAL:CG2	2.51	0.40
1:D:313:LEU:O	1:D:338:ASN:HA	2.21	0.40
1:A:8:ASN:HB3	1:A:15:PHE:HA	2.02	0.40
1:C:300:LEU:HD23	1:C:300:LEU:HA	1.87	0.40
1:B:207:ARG:CG	3:B:523:HOH:O	2.68	0.40
1:A:205:LEU:HA	1:A:206:PRO:HD3	1.93	0.40
1:B:7:PHE:HA	1:B:22:LEU:HD12	2.03	0.40
1:A:241:VAL:O	1:A:241:VAL:HG13	2.21	0.40
1:A:248:GLY:C	1:A:250:HIS:HD2	2.25	0.40
1:A:149:ALA:O	1:A:151:LYS:HE3	2.21	0.40
1:D:144:GLY:C	1:D:145:LYS:CG	2.88	0.40
1:B:241:VAL:HG21	1:B:284:TYR:CD1	2.56	0.40
1:C:173:LYS:HD2	1:E:287:ASP:OD1	2.22	0.40
1:F:250:HIS:CE1	1:F:344:TYR:HB3	2.57	0.40
1:C:218:ASP:OD1	1:F:225:LYS:HE2	2.22	0.40
1:A:24:VAL:HG13	1:A:33:VAL:HG22	2.03	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

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	338/349 (97%)	317 (94%)	14 (4%)	7 (2%)	9	14
1	B	338/349 (97%)	319 (94%)	17 (5%)	2 (1%)	30	50
1	C	338/349 (97%)	321 (95%)	14 (4%)	3 (1%)	21	37
1	D	338/349 (97%)	318 (94%)	17 (5%)	3 (1%)	21	37
1	E	338/349 (97%)	323 (96%)	13 (4%)	2 (1%)	30	50
1	F	338/349 (97%)	320 (95%)	16 (5%)	2 (1%)	30	50
All	All	2028/2094 (97%)	1918 (95%)	91 (4%)	19 (1%)	21	37

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%)	273 (92%)	25 (8%)	14	25
1	B	298/304 (98%)	273 (92%)	25 (8%)	14	25
1	C	298/304 (98%)	272 (91%)	26 (9%)	13	24
1	D	298/304 (98%)	271 (91%)	27 (9%)	12	22
1	E	298/304 (98%)	273 (92%)	25 (8%)	14	25
1	F	298/304 (98%)	279 (94%)	19 (6%)	22	39
All	All	1788/1824 (98%)	1641 (92%)	147 (8%)	14	27

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	34	ARG
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	189	ASP
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

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Mol	Chain	Res	Type
1	A	311	LEU
1	A	322	VAL
1	A	342	THR
1	B	24	VAL
1	B	34	ARG
1	B	71	ILE
1	B	84	VAL
1	B	111	VAL
1	B	128	LEU
1	B	134	LEU
1	B	142	THR
1	B	146	SER
1	B	147	LEU
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	320	HIS
1	B	342	THR
1	C	24	VAL
1	C	34	ARG
1	C	47	THR
1	C	71	ILE
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	152	LEU
1	C	153	ASN
1	C	165	VAL
1	C	172	ILE

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Mol	Chain	Res	Type
1	C	218	ASP
1	C	233	PHE
1	C	241	VAL
1	C	244	THR
1	C	252	LEU
1	C	300	LEU
1	C	302	ASP
1	C	311	LEU
1	C	313	LEU
1	C	320	HIS
1	C	322	VAL
1	C	342	THR
1	D	24	VAL
1	D	34	ARG
1	D	47	THR
1	D	71	ILE
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	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	302	ASP
1	D	311	LEU
1	D	320	HIS
1	D	322	VAL
1	D	342	THR
1	E	24	VAL
1	E	47	THR
1	E	71	ILE

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Mol	Chain	Res	Type
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	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	302	ASP
1	E	311	LEU
1	E	313	LEU
1	E	342	THR
1	F	24	VAL
1	F	34	ARG
1	F	47	THR
1	F	71	ILE
1	F	111	VAL
1	F	128	LEU
1	F	134	LEU
1	F	147	LEU
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	342	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	174	ASN
1	A	190	HIS
1	A	216	ASN
1	A	250	HIS
1	A	320	HIS
1	B	153	ASN
1	B	174	ASN
1	B	190	HIS
1	B	216	ASN
1	B	320	HIS
1	C	11	ASN
1	C	153	ASN
1	C	174	ASN
1	C	190	HIS
1	C	216	ASN
1	C	250	HIS
1	C	320	HIS
1	D	153	ASN
1	D	174	ASN
1	D	190	HIS
1	D	216	ASN
1	D	320	HIS
1	E	153	ASN
1	E	174	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	190	HIS
1	F	216	ASN
1	F	320	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	A	401	-	4,4,4	0.28	0	6,6,6	0.25	0
2	PO4	B	401	-	4,4,4	0.53	0	6,6,6	0.34	0
2	PO4	C	401	-	4,4,4	0.65	0	6,6,6	0.27	0
2	PO4	D	401	-	4,4,4	1.04	0	6,6,6	0.28	0
2	PO4	E	401	-	4,4,4	0.40	0	6,6,6	0.25	0
2	PO4	F	401	-	4,4,4	1.05	0	6,6,6	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	401	-	-	0/0/0/0	0/0/0/0
2	PO4	B	401	-	-	0/0/0/0	0/0/0/0
2	PO4	C	401	-	-	0/0/0/0	0/0/0/0
2	PO4	D	401	-	-	0/0/0/0	0/0/0/0
2	PO4	E	401	-	-	0/0/0/0	0/0/0/0
2	PO4	F	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.53	31 (9%) 11 12	30, 46, 82, 102	0
1	B	342/349 (97%)	0.65	39 (11%) 7 6	28, 48, 84, 130	0
1	C	342/349 (97%)	0.18	5 (1%) 76 79	28, 43, 80, 101	0
1	D	342/349 (97%)	0.36	14 (4%) 41 46	27, 44, 79, 113	0
1	E	342/349 (97%)	0.19	7 (2%) 68 72	28, 45, 80, 112	0
1	F	342/349 (97%)	0.08	4 (1%) 81 83	28, 45, 81, 109	0
All	All	2052/2094 (97%)	0.33	100 (4%) 33 38	27, 45, 81, 130	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	228	LEU	8.9
1	A	144	GLY	8.8
1	D	144	GLY	8.2
1	D	146	SER	7.0
1	D	142	THR	5.8
1	B	338	ASN	5.7
1	A	165	VAL	5.2
1	B	334	TRP	5.2
1	C	316	VAL	4.8
1	F	144	GLY	4.6
1	A	147	LEU	4.5
1	B	309	LYS	4.4
1	B	223	ILE	4.3
1	B	147	LEU	4.3
1	D	141	LYS	4.1
1	E	231	PHE	4.0
1	A	314	THR	3.8
1	B	134	LEU	3.8
1	A	150	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	139	ALA	3.7
1	B	227	GLY	3.6
1	F	143	GLY	3.6
1	B	339	ALA	3.6
1	B	333	LEU	3.5
1	B	311	LEU	3.5
1	A	179	VAL	3.5
1	B	307	VAL	3.5
1	A	149	ALA	3.5
1	B	230	ASP	3.4
1	A	140	VAL	3.3
1	B	183	LYS	3.3
1	E	313	LEU	3.3
1	B	143	GLY	3.2
1	B	107	PHE	3.2
1	D	149	ALA	3.2
1	B	214	PHE	3.1
1	B	316	VAL	3.0
1	B	236	VAL	3.0
1	A	321	GLU	2.9
1	C	334	TRP	2.9
1	D	334	TRP	2.9
1	A	332	MET	2.9
1	B	226	TYR	2.9
1	B	221	VAL	2.9
1	D	145	LYS	2.8
1	B	109	GLU	2.8
1	A	335	CYS	2.8
1	E	343	PHE	2.8
1	A	320	HIS	2.8
1	D	140	VAL	2.7
1	A	151	LYS	2.7
1	A	120	GLN	2.7
1	E	171	ASN	2.6
1	B	181	VAL	2.6
1	B	335	CYS	2.6
1	B	144	GLY	2.6
1	A	191	TYR	2.6
1	E	315	VAL	2.5
1	C	172	ILE	2.5
1	A	146	SER	2.5
1	A	182	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	320	HIS	2.4
1	B	165	VAL	2.4
1	A	188	VAL	2.4
1	A	315	VAL	2.4
1	E	309	LYS	2.4
1	A	115	TYR	2.4
1	A	148	PRO	2.4
1	B	110	ASP	2.4
1	C	335	CYS	2.3
1	A	145	LYS	2.3
1	B	340	VAL	2.3
1	D	171	ASN	2.3
1	B	341	ALA	2.3
1	B	215	LEU	2.3
1	A	128	LEU	2.2
1	C	144	GLY	2.2
1	A	123	TYR	2.2
1	E	142	THR	2.2
1	A	194	PHE	2.2
1	B	128	LEU	2.2
1	B	142	THR	2.1
1	D	150	ILE	2.1
1	B	328	PRO	2.1
1	A	344	TYR	2.1
1	B	180	TYR	2.1
1	B	220	GLY	2.1
1	F	311	LEU	2.1
1	B	186	LYS	2.1
1	B	172	ILE	2.1
1	A	236	VAL	2.1
1	A	132	ALA	2.1
1	D	340	VAL	2.1
1	D	147	LEU	2.1
1	A	183	LYS	2.1
1	A	340	VAL	2.0
1	A	190	HIS	2.0
1	F	244	THR	2.0
1	B	120	GLN	2.0
1	B	141	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PO4	F	401	5/5	0.85	0.15	-0.40	45,47,57,87	0
2	PO4	A	401	5/5	0.92	0.15	-0.68	60,63,80,99	0
2	PO4	B	401	5/5	0.87	0.15	-0.86	56,57,72,107	0
2	PO4	E	401	5/5	0.94	0.12	-1.29	51,65,75,85	0
2	PO4	D	401	5/5	0.90	0.12	-1.70	39,39,63,75	0
2	PO4	C	401	5/5	0.93	0.09	-2.63	42,45,63,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.