



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:09 PM GMT

PDB ID : 3W9T
Title : pore-forming CEL-III
Authors : Unno, H.; Goda, S.; Hatakeyama, T.
Deposited on : 2013-04-16
Resolution : 2.90 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

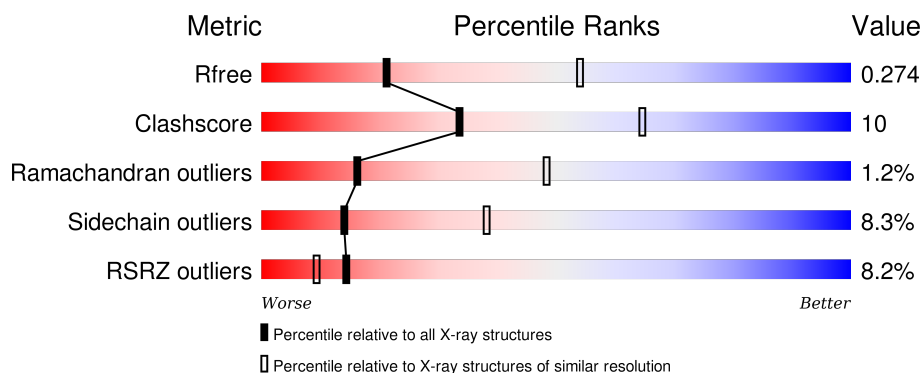
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



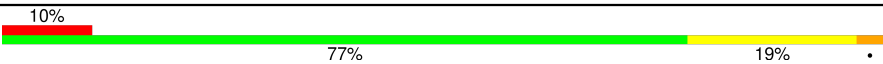

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	432	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>••</div> </div> </div>
1	B	432	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>•</div> </div> </div>
1	C	432	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>••</div> </div> </div>
1	D	432	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div>
1	E	432	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	432	
1	G	432	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	W9T	E	505	-	-	-	X
2	W9T	G	505	-	-	-	X
3	CA	C	1014	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24175 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 Hemolytic lectin CEL-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	C	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	G	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	B	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	F	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	E	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	D	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	-	EXPRESSION TAG	UNP Q868M7
A	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
A	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
A	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
A	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
A	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
A	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
A	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
A	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
A	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
A	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
A	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
A	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
A	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
C	1	PCA	-	EXPRESSION TAG	UNP Q868M7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
C	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
C	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
C	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
C	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
C	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
C	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
C	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
C	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
C	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
C	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
C	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
C	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
G	1	PCA	-	EXPRESSION TAG	UNP Q868M7
G	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
G	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
G	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
G	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
G	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
G	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
G	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
G	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
G	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
G	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
G	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
G	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
G	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
B	1	PCA	-	EXPRESSION TAG	UNP Q868M7
B	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
B	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
B	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
B	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
B	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
B	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
B	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
B	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
B	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
B	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
B	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
B	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
B	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
F	1	PCA	-	EXPRESSION TAG	UNP Q868M7

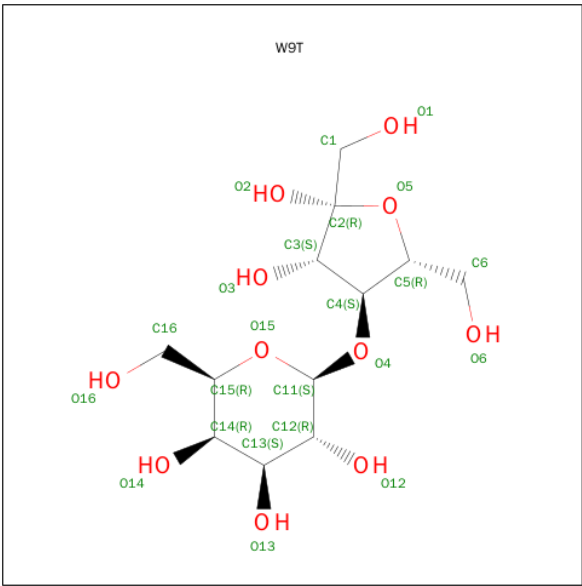
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Chain	Residue	Modelled	Actual	Comment	Reference
F	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
F	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
F	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
F	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
F	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
F	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
F	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
F	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
F	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
F	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
F	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
F	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
F	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
E	1	PCA	-	EXPRESSION TAG	UNP Q868M7
E	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
E	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
E	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
E	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
E	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
E	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
E	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
E	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
E	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
E	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
E	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
E	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
E	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
D	1	PCA	-	EXPRESSION TAG	UNP Q868M7
D	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
D	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
D	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
D	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
D	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
D	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
D	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
D	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
D	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
D	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
D	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
D	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
D	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7

- Molecule 2 is 4-O-BETA-D-GALACTOPYRANOSYL-BETA-D-FRUCTOFURANOSE

(three-letter code: W9T) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	G	1	Total	C	O	0	0
			23	12	11		
2	G	1	Total	C	O	0	0
			23	12	11		
2	G	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			23	12	11		
2	G	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	6	Total	Ca	0	0
			6	6		
3	D	6	Total	Ca	0	0
			6	6		
3	E	7	Total	Ca	0	0
			7	7		
3	B	6	Total	Ca	0	0
			6	6		
3	C	7	Total	Ca	0	0
			7	7		
3	A	6	Total	Ca	0	0
			6	6		
3	F	6	Total	Ca	0	0
			6	6		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	F	2	Total	Mg	0	0
			2	2		

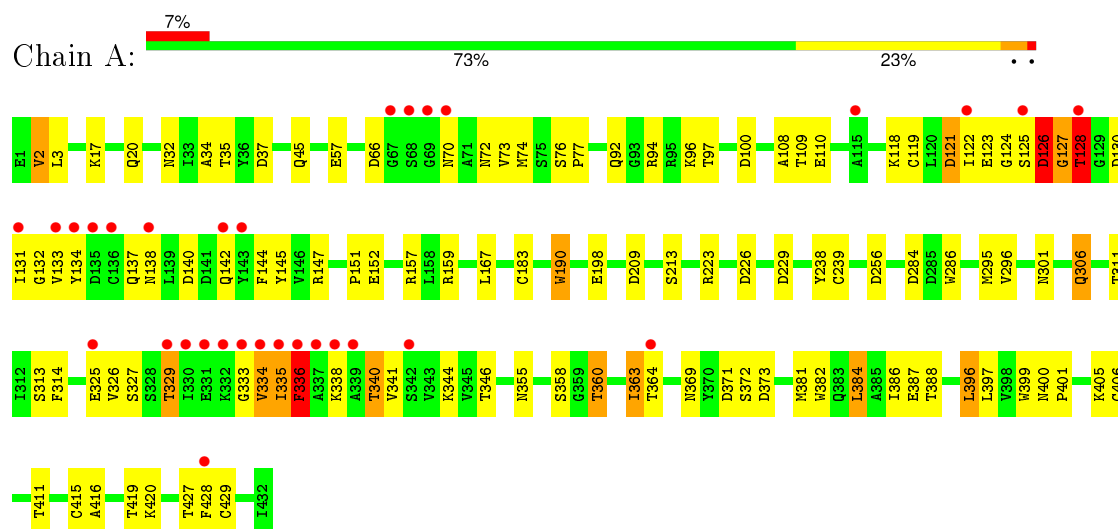
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total 10	O 10	0	0
5	C	9	Total 9	O 9	0	0
5	G	5	Total 5	O 5	0	0
5	B	14	Total 14	O 14	0	0
5	F	13	Total 13	O 13	0	0
5	E	10	Total 10	O 10	0	0
5	D	14	Total 14	O 14	0	0

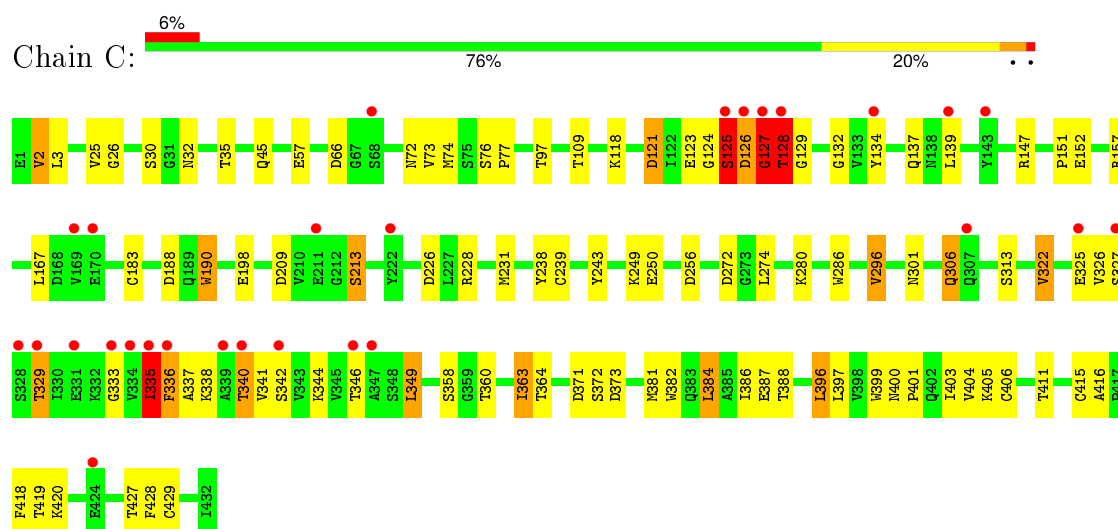
3 Residue-property plots

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.

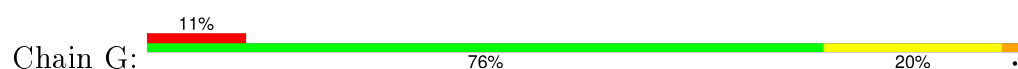
• Molecule 1: Hemolytic lectin CEL-III

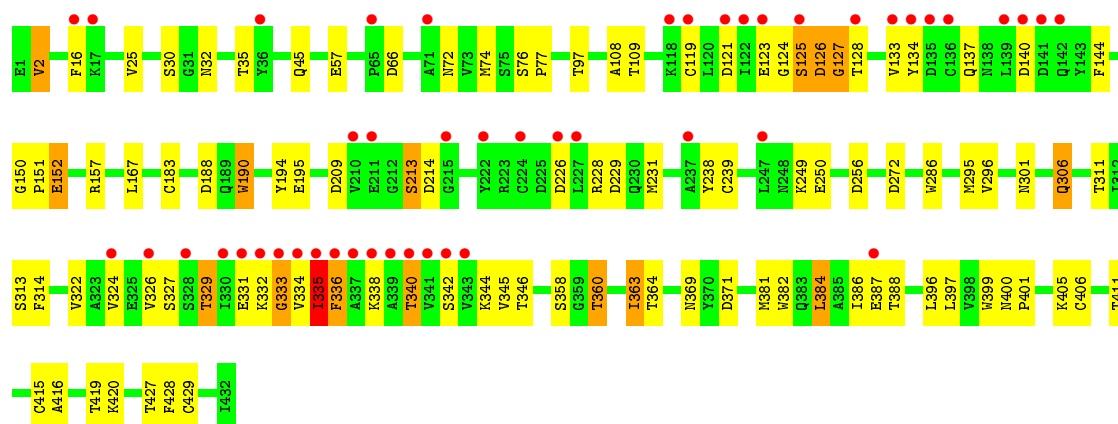


• Molecule 1: Hemolytic lectin CEL-III

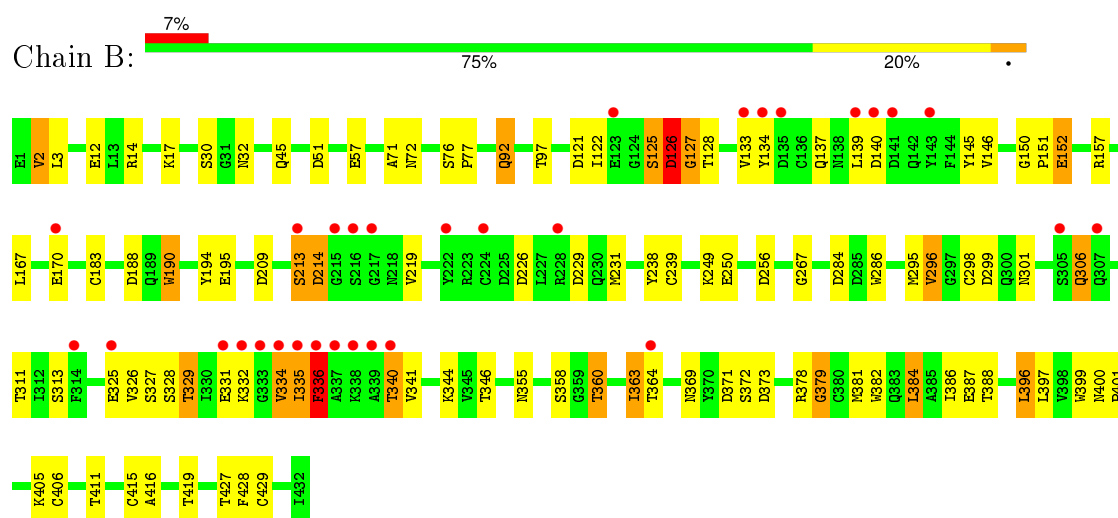


• Molecule 1: Hemolytic lectin CEL-III

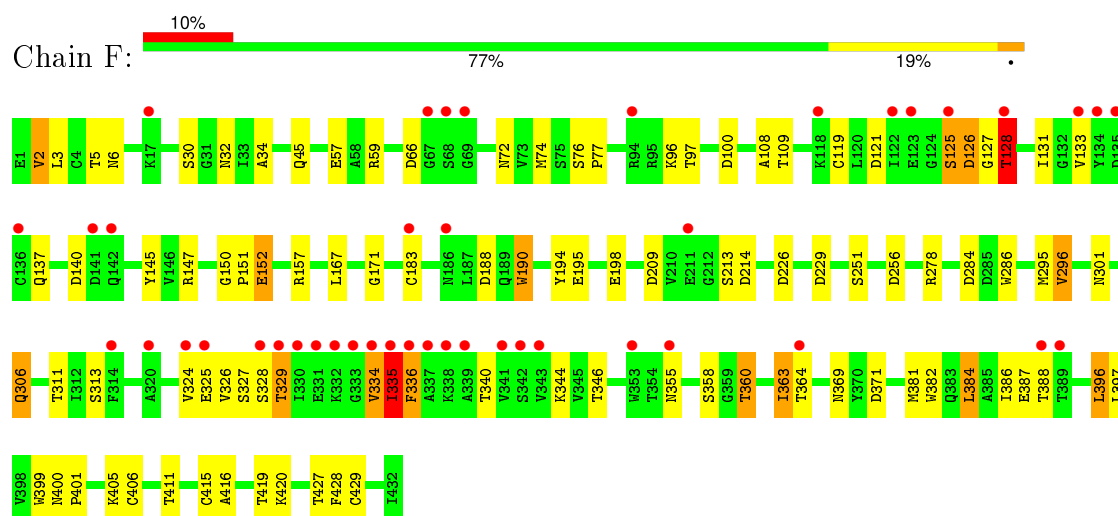




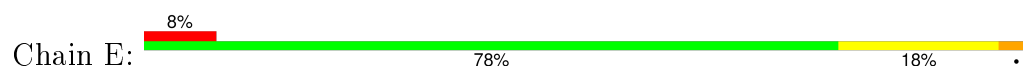
• Molecule 1: Hemolytic lectin CEL-III

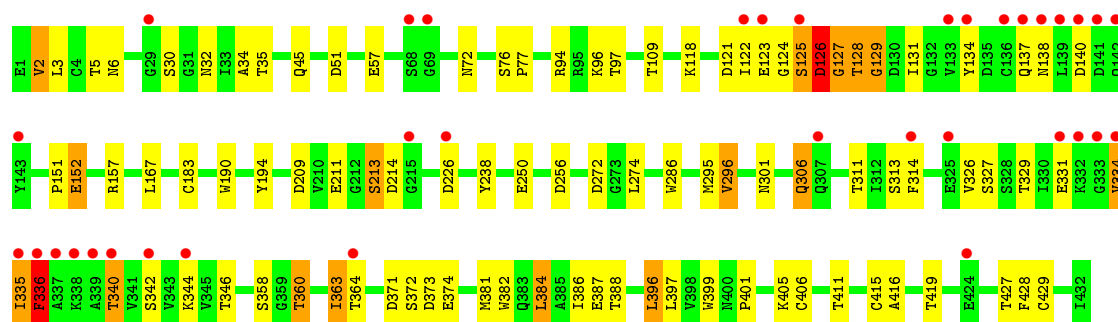


• Molecule 1: Hemolytic lectin CEL-III

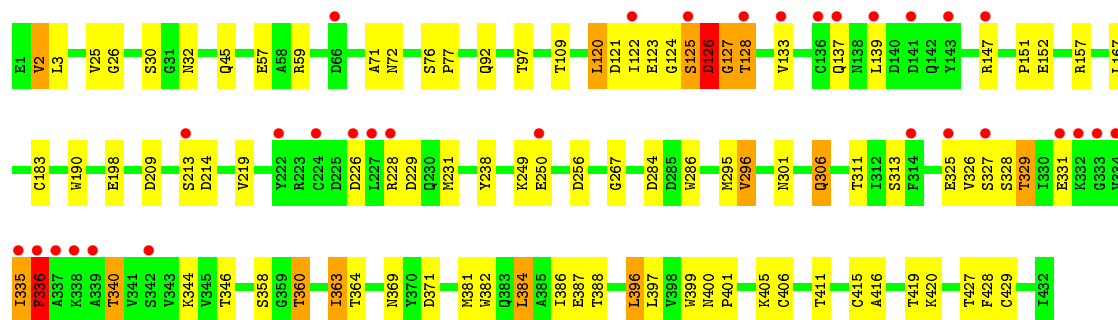
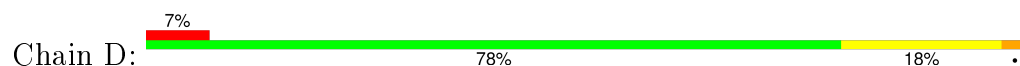


• Molecule 1: Hemolytic lectin CEL-III





• Molecule 1: Hemolytic lectin CEL-III



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.80Å 228.65Å 133.02Å 90.00° 127.13° 90.00°	Depositor
Resolution (Å)	48.20 – 2.90 48.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.20-2.90) 98.4 (48.20-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.239 , 0.273 0.239 , 0.274	Depositor DCC
R_{free} test set	5793 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
Estimated twinning fraction	0.000 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 113677 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24175	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, W9T, PCA, MG

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	0.47	1/3366 (0.0%)	0.70	3/4566 (0.1%)
1	B	0.47	1/3366 (0.0%)	0.72	4/4566 (0.1%)
1	C	0.46	0/3366	0.71	5/4566 (0.1%)
1	D	0.45	0/3366	0.68	2/4566 (0.0%)
1	E	0.47	0/3366	0.69	2/4566 (0.0%)
1	F	0.49	0/3366	0.70	2/4566 (0.0%)
1	G	0.45	0/3366	0.71	1/4566 (0.0%)
All	All	0.47	2/23562 (0.0%)	0.70	19/31962 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	3
1	G	0	4
All	All	0	25

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASP	CG-OD2	-7.12	1.08	1.25
1	B	379	GLY	N-CA	-5.95	1.37	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASP	CB-CG-OD1	13.30	130.27	118.30
1	C	128	THR	N-CA-C	-10.58	82.44	111.00
1	B	378	ARG	C-N-CA	9.70	142.68	122.30
1	A	126	ASP	OD1-CG-OD2	-8.37	107.39	123.30
1	B	378	ARG	CA-C-N	7.94	132.07	116.20
1	C	349	LEU	CA-CB-CG	6.93	131.23	115.30
1	E	129	GLY	N-CA-C	6.81	130.11	113.10
1	B	378	ARG	O-C-N	-6.64	111.91	123.20
1	C	349	LEU	CB-CG-CD1	6.01	121.23	111.00
1	D	120	LEU	CB-CG-CD2	5.99	121.17	111.00
1	E	396	LEU	CA-CB-CG	5.77	128.56	115.30
1	B	396	LEU	CA-CB-CG	5.74	128.50	115.30
1	D	396	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	396	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	396	LEU	CA-CB-CG	5.26	127.40	115.30
1	G	2	VAL	CG1-CB-CG2	5.20	119.23	110.90
1	F	2	VAL	CG1-CB-CG2	5.18	119.19	110.90
1	F	396	LEU	CA-CB-CG	5.08	127.00	115.30
1	C	322	VAL	CG1-CB-CG2	5.02	118.94	110.90

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	PRO	Peptide
1	A	335	ILE	Peptide
1	B	126	ASP	Peptide
1	B	127	GLY	Peptide
1	B	151	PRO	Peptide
1	B	335	ILE	Peptide
1	C	125	SER	Peptide
1	C	127	GLY	Peptide
1	C	151	PRO	Peptide
1	C	335	ILE	Peptide
1	D	126	ASP	Peptide
1	D	127	GLY	Peptide
1	D	151	PRO	Peptide
1	D	335	ILE	Peptide
1	E	126	ASP	Peptide
1	E	127	GLY	Peptide
1	E	151	PRO	Peptide
1	E	335	ILE	Peptide
1	F	127	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	F	151	PRO	Peptide
1	F	335	ILE	Peptide
1	G	127	GLY	Peptide
1	G	151	PRO	Peptide
1	G	332	LYS	Peptide
1	G	335	ILE	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	3313	0	3083	92	2
1	B	3313	0	3082	90	1
1	C	3313	0	3083	90	0
1	D	3313	0	3082	69	1
1	E	3313	0	3083	71	1
1	F	3313	0	3083	77	0
1	G	3313	0	3083	79	0
2	A	115	0	107	3	0
2	B	138	0	128	6	0
2	C	115	0	106	8	0
2	D	115	0	106	4	0
2	E	138	0	129	11	0
2	F	115	0	108	8	0
2	G	115	0	105	5	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	7	0	0	0	2
3	D	6	0	0	0	0
3	E	7	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	2	0	0	0	0
5	A	10	0	0	1	0
5	B	14	0	0	0	0
5	C	9	0	0	1	0
5	D	14	0	0	0	0
5	E	10	0	0	0	0
5	F	13	0	0	0	0
5	G	5	0	0	0	0
All	All	24175	0	22368	472	4

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 10.

All (472) 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:C:340:THR:HG23	1:B:329:THR:HG23	1.12	1.07
1:B:125:SER:HB3	1:B:139:LEU:HD13	1.39	1.05
1:E:340:THR:HG23	1:D:329:THR:HG23	1.42	1.02
2:E:506:W9T:O15	2:E:506:W9T:H17	1.61	0.97
1:E:6:ASN:HB2	2:E:506:W9T:H3	1.50	0.92
1:D:125:SER:O	1:D:126:ASP:HB2	1.67	0.92
1:C:340:THR:CG2	1:B:329:THR:HG23	2.00	0.91
1:C:2:VAL:HG13	1:B:238:TYR:HA	1.52	0.88
1:A:238:TYR:HA	1:B:2:VAL:HG13	1.53	0.88
1:C:399:TRP:HE1	1:B:306:GLN:HE22	1.20	0.88
1:E:344:LYS:HB3	1:D:325:GLU:HB3	1.56	0.88
1:G:406:CYS:H	1:F:301:ASN:HD22	1.21	0.88
1:E:340:THR:CG2	1:D:329:THR:HG23	2.04	0.87
1:E:406:CYS:H	1:D:301:ASN:ND2	1.74	0.86
1:A:2:VAL:HG13	1:G:238:TYR:HA	1.56	0.86
1:C:399:TRP:HE1	1:B:306:GLN:NE2	1.72	0.85
1:B:125:SER:O	1:B:126:ASP:HB2	1.76	0.85
1:G:344:LYS:HB3	1:F:325:GLU:HB3	1.59	0.84
1:E:406:CYS:H	1:D:301:ASN:HD22	1.24	0.84
1:C:419:THR:CG2	1:C:429:CYS:HB3	2.09	0.83
1:A:399:TRP:HE1	1:G:306:GLN:NE2	1.77	0.83
1:C:416:ALA:O	1:C:419:THR:HB	1.79	0.82
1:E:2:VAL:HG13	1:D:238:TYR:HA	1.62	0.82
1:G:406:CYS:H	1:F:301:ASN:ND2	1.76	0.82
1:D:416:ALA:O	1:D:419:THR:HB	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:THR:HG21	1:C:401:PRO:O	1.80	0.81
1:E:419:THR:CG2	1:E:429:CYS:HB3	2.10	0.81
1:F:416:ALA:O	1:F:419:THR:HB	1.81	0.80
1:B:416:ALA:O	1:B:419:THR:HB	1.82	0.80
1:B:125:SER:O	1:B:126:ASP:CB	2.31	0.79
1:G:128:THR:O	1:G:128:THR:HG22	1.80	0.79
1:A:419:THR:CG2	1:A:429:CYS:HB3	2.13	0.79
1:B:388:THR:HG21	1:B:401:PRO:O	1.81	0.79
1:C:238:TYR:HA	1:D:2:VAL:HG13	1.65	0.79
1:A:399:TRP:HE1	1:G:306:GLN:HE22	1.29	0.79
1:D:419:THR:CG2	1:D:429:CYS:HB3	2.11	0.79
1:B:419:THR:CG2	1:B:429:CYS:HB3	2.13	0.79
1:G:125:SER:O	1:G:126:ASP:HB2	1.81	0.78
1:G:35:THR:OG1	1:G:128:THR:O	2.01	0.78
1:D:388:THR:HG21	1:D:401:PRO:O	1.82	0.78
1:E:388:THR:HG21	1:E:401:PRO:O	1.84	0.78
1:G:388:THR:HG21	1:G:401:PRO:O	1.84	0.78
1:G:419:THR:CG2	1:G:429:CYS:HB3	2.14	0.78
1:A:388:THR:HG21	1:A:401:PRO:O	1.83	0.77
1:A:301:ASN:HD22	1:B:406:CYS:H	1.32	0.77
1:F:419:THR:CG2	1:F:429:CYS:HB3	2.14	0.77
1:A:124:GLY:H	2:A:1002:W9T:H9	1.49	0.77
1:A:416:ALA:O	1:A:419:THR:HB	1.85	0.77
1:F:399:TRP:HE1	1:E:306:GLN:NE2	1.84	0.76
1:C:406:CYS:H	1:B:301:ASN:ND2	1.84	0.76
1:G:416:ALA:O	1:G:419:THR:HB	1.86	0.76
1:C:340:THR:HG23	1:B:329:THR:CG2	2.07	0.76
1:F:399:TRP:HE1	1:E:306:GLN:HE22	1.33	0.76
1:G:340:THR:O	1:F:328:SER:HB2	1.85	0.75
1:G:134:TYR:CE1	2:G:505:W9T:H4	2.22	0.75
1:E:399:TRP:HE1	1:D:306:GLN:HE22	1.35	0.74
1:F:388:THR:HG21	1:F:401:PRO:O	1.87	0.74
1:D:125:SER:O	1:D:126:ASP:CB	2.36	0.73
1:E:416:ALA:O	1:E:419:THR:HB	1.89	0.73
1:F:125:SER:O	1:F:126:ASP:HB2	1.89	0.73
1:A:306:GLN:NE2	1:B:399:TRP:HE1	1.88	0.72
1:A:35:THR:OG1	1:A:128:THR:HB	1.89	0.72
1:C:124:GLY:HA2	2:C:1004:W9T:H9	1.72	0.72
1:A:306:GLN:HE22	1:B:399:TRP:HE1	1.38	0.72
1:C:125:SER:O	1:C:126:ASP:HB2	1.91	0.71
1:A:313:SER:HB3	1:A:358:SER:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:GLY:HA2	2:E:505:W9T:H9	1.73	0.71
1:B:313:SER:HB3	1:B:358:SER:HB3	1.71	0.71
1:D:384:LEU:HD13	1:D:386:ILE:HG12	1.72	0.70
1:C:399:TRP:CD1	1:B:296:VAL:HG22	2.26	0.70
1:D:313:SER:HB3	1:D:358:SER:HB3	1.74	0.70
1:C:344:LYS:HB3	1:B:325:GLU:HB3	1.74	0.70
1:E:399:TRP:HE1	1:D:306:GLN:NE2	1.90	0.70
1:C:337:ALA:HA	1:B:332:LYS:HA	1.73	0.70
1:F:313:SER:HB3	1:F:358:SER:HB3	1.74	0.69
1:D:124:GLY:HA2	2:D:506:W9T:H9	1.74	0.69
1:E:125:SER:O	1:E:126:ASP:HB2	1.92	0.69
1:F:171:GLY:HA2	2:F:503:W9T:O4	1.92	0.69
1:A:301:ASN:ND2	1:B:406:CYS:H	1.90	0.69
1:C:338:LYS:N	1:B:331:GLU:O	2.22	0.69
2:E:506:W9T:O15	2:E:506:W9T:C3	2.40	0.68
1:G:306:GLN:HG2	1:G:381:MET:HE1	1.75	0.68
1:E:313:SER:HB3	1:E:358:SER:HB3	1.74	0.68
1:G:313:SER:HB3	1:G:358:SER:HB3	1.76	0.68
1:C:301:ASN:HB3	1:D:369:ASN:O	1.93	0.68
1:G:399:TRP:HE1	1:F:306:GLN:HE22	1.41	0.68
1:B:384:LEU:HD13	1:B:386:ILE:HG12	1.75	0.68
1:B:51:ASP:HB3	2:B:513:W9T:H12	1.74	0.68
1:A:73:VAL:HG23	1:A:132:GLY:HA2	1.75	0.67
1:D:306:GLN:HG2	1:D:381:MET:HE1	1.76	0.67
1:E:384:LEU:HD13	1:E:386:ILE:HG12	1.74	0.67
1:G:327:SER:HB3	1:G:344:LYS:HG3	1.76	0.67
1:F:306:GLN:HG2	1:F:381:MET:HE1	1.77	0.67
1:C:76:SER:HB2	1:C:77:PRO:HD2	1.76	0.66
1:G:399:TRP:HE1	1:F:306:GLN:NE2	1.93	0.66
1:E:76:SER:HB2	1:E:77:PRO:HD2	1.76	0.66
1:D:76:SER:HB2	1:D:77:PRO:HD2	1.76	0.66
1:G:76:SER:HB2	1:G:77:PRO:HD2	1.77	0.66
1:F:327:SER:HB3	1:F:344:LYS:HG3	1.78	0.66
1:A:124:GLY:N	2:A:1002:W9T:H9	2.11	0.66
1:A:327:SER:HB3	1:A:344:LYS:HG3	1.77	0.65
1:C:384:LEU:HD13	1:C:386:ILE:HG12	1.78	0.65
1:A:384:LEU:HD13	1:A:386:ILE:HG12	1.78	0.65
1:A:76:SER:HB2	1:A:77:PRO:HD2	1.77	0.65
1:C:306:GLN:HE22	1:D:399:TRP:HE1	1.44	0.65
1:E:306:GLN:HG2	1:E:381:MET:HE1	1.77	0.64
1:B:327:SER:HB3	1:B:344:LYS:HG3	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:384:LEU:HD13	1:F:386:ILE:HG12	1.78	0.64
1:C:134:TYR:CE1	2:C:1004:W9T:H4	2.33	0.64
2:F:512:W9T:O15	2:F:512:W9T:H17	1.97	0.64
1:A:336:PHE:HB2	1:G:334:VAL:CG1	2.28	0.64
1:A:119:CYS:O	1:A:133:VAL:HA	1.98	0.64
1:B:134:TYR:CE1	2:B:504:W9T:H4	2.33	0.64
1:D:327:SER:HB3	1:D:344:LYS:HG3	1.79	0.64
1:A:70:ASN:ND2	1:A:134:TYR:CE1	2.66	0.63
1:B:76:SER:HB2	1:B:77:PRO:HD2	1.79	0.63
1:B:306:GLN:HG2	1:B:381:MET:HE1	1.80	0.63
1:G:384:LEU:HD13	1:G:386:ILE:HG12	1.80	0.63
1:G:340:THR:CG2	1:F:329:THR:HG23	2.29	0.62
1:A:118:LYS:HB2	1:A:133:VAL:HB	1.81	0.62
1:C:342:SER:HB2	1:B:327:SER:OG	1.99	0.62
1:E:342:SER:HB2	1:D:327:SER:OG	2.00	0.61
2:E:506:W9T:O13	2:E:506:W9T:O15	2.06	0.61
1:G:340:THR:HG23	1:F:329:THR:HG23	1.81	0.61
1:F:76:SER:HB2	1:F:77:PRO:HD2	1.81	0.61
1:E:327:SER:HB3	1:E:344:LYS:HG3	1.82	0.61
1:F:128:THR:HG22	1:F:128:THR:O	1.99	0.61
1:F:77:PRO:HB3	1:E:272:ASP:HA	1.83	0.61
1:B:17:LYS:HD2	1:B:140:ASP:HB2	1.82	0.60
1:C:406:CYS:H	1:B:301:ASN:HD22	1.48	0.60
1:B:71:ALA:O	1:B:133:VAL:HG22	2.01	0.60
1:F:363:ILE:HD11	1:F:399:TRP:HD1	1.67	0.60
1:E:363:ILE:HD11	1:E:399:TRP:HD1	1.66	0.59
1:C:125:SER:O	1:C:126:ASP:CB	2.49	0.59
1:A:20:GLN:NE2	5:A:1102:HOH:O	2.34	0.59
1:F:171:GLY:HA2	2:F:503:W9T:C4	2.32	0.59
1:C:306:GLN:NE2	1:D:399:TRP:HE1	2.00	0.59
1:C:301:ASN:HD22	1:D:406:CYS:H	1.51	0.59
1:C:313:SER:HB3	1:C:358:SER:HB3	1.84	0.58
1:A:96:LYS:HE3	1:A:140:ASP:OD1	2.03	0.58
1:E:51:ASP:HB3	2:E:506:W9T:H4	1.85	0.58
1:G:399:TRP:CD1	1:F:296:VAL:HG22	2.38	0.58
1:F:45:GLN:HB3	1:F:57:GLU:HG3	1.85	0.58
1:F:399:TRP:CD1	1:E:296:VAL:HG22	2.39	0.58
1:A:336:PHE:HB2	1:G:334:VAL:HG13	1.86	0.58
1:F:355:ASN:HB3	1:E:314:PHE:CD1	2.39	0.57
1:E:399:TRP:CD1	1:D:296:VAL:HG22	2.40	0.57
1:G:125:SER:O	1:G:126:ASP:CB	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ASN:ND2	1:D:406:CYS:H	2.02	0.57
1:C:239:CYS:O	1:D:2:VAL:HG22	2.04	0.57
1:F:45:GLN:CB	1:F:57:GLU:HG3	2.35	0.57
1:C:125:SER:HB3	1:C:139:LEU:HD13	1.86	0.57
1:A:406:CYS:H	1:G:301:ASN:ND2	2.03	0.57
1:G:124:GLY:HA2	2:G:505:W9T:H9	1.86	0.57
1:A:406:CYS:H	1:G:301:ASN:HD22	1.51	0.56
1:F:334:VAL:HG13	1:F:335:ILE:HD12	1.87	0.56
1:C:341:VAL:HG12	1:B:328:SER:HB2	1.86	0.56
1:G:313:SER:HB3	1:G:358:SER:CB	2.36	0.56
1:D:335:ILE:O	1:D:336:PHE:HD2	1.87	0.56
1:B:313:SER:HB3	1:B:358:SER:CB	2.35	0.56
1:A:2:VAL:HG22	1:G:239:CYS:O	2.06	0.56
1:C:418:PHE:CZ	1:B:379:GLY:HA3	2.41	0.56
1:G:306:GLN:CG	1:G:381:MET:HE1	2.34	0.56
1:C:327:SER:HB3	1:C:344:LYS:HG3	1.87	0.56
1:E:123:GLU:HA	2:E:505:W9T:H3	1.86	0.56
1:D:363:ILE:HD11	1:D:399:TRP:HD1	1.70	0.56
1:A:126:ASP:OD2	1:A:128:THR:HG23	2.06	0.56
1:A:335:ILE:O	1:A:336:PHE:HD2	1.89	0.56
1:B:335:ILE:O	1:B:336:PHE:HD2	1.89	0.56
1:G:406:CYS:N	1:F:301:ASN:HD22	1.99	0.56
1:D:415:CYS:HB3	1:D:419:THR:HG22	1.88	0.56
1:E:335:ILE:O	1:E:336:PHE:HD2	1.89	0.55
1:E:340:THR:HG23	1:D:329:THR:CG2	2.28	0.55
1:A:363:ILE:HD11	1:A:399:TRP:HD1	1.72	0.55
1:B:134:TYR:CZ	2:B:504:W9T:H4	2.41	0.55
1:F:415:CYS:HB3	1:F:419:THR:HG22	1.88	0.55
1:A:118:LYS:CB	1:A:133:VAL:HB	2.37	0.55
1:A:108:ALA:HA	1:A:144:PHE:O	2.06	0.55
1:D:125:SER:HB3	1:D:139:LEU:HD13	1.88	0.55
1:E:313:SER:HB3	1:E:358:SER:CB	2.38	0.55
1:F:306:GLN:CG	1:F:381:MET:HE1	2.37	0.55
1:A:119:CYS:N	1:A:134:TYR:O	2.37	0.54
1:G:345:VAL:HG22	1:F:324:VAL:HG22	1.89	0.54
1:B:415:CYS:HB3	1:B:419:THR:HG22	1.88	0.54
1:B:334:VAL:HG13	1:B:335:ILE:HD12	1.90	0.54
1:F:313:SER:HB3	1:F:358:SER:CB	2.37	0.54
1:E:371:ASP:OD2	1:E:405:LYS:NZ	2.40	0.54
1:E:45:GLN:CB	1:E:57:GLU:HG3	2.38	0.54
1:C:306:GLN:HG2	1:C:381:MET:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLN:HG2	1:A:381:MET:HE1	1.90	0.54
1:G:415:CYS:HB3	1:G:419:THR:HG22	1.90	0.54
1:D:71:ALA:O	1:D:133:VAL:HG22	2.08	0.54
1:B:45:GLN:HB3	1:B:57:GLU:HG3	1.90	0.54
1:A:415:CYS:HB3	1:A:419:THR:HG22	1.90	0.54
1:B:363:ILE:HD11	1:B:399:TRP:HD1	1.72	0.54
1:C:124:GLY:CA	2:C:1004:W9T:H9	2.38	0.54
1:E:45:GLN:HB3	1:E:57:GLU:HG3	1.90	0.54
1:C:35:THR:OG1	1:C:128:THR:HG22	2.09	0.53
1:C:35:THR:OG1	1:C:129:GLY:N	2.41	0.53
1:F:406:CYS:H	1:E:301:ASN:HD22	1.55	0.53
1:A:110:GLU:HA	1:A:142:GLN:O	2.08	0.53
1:E:340:THR:O	1:D:328:SER:HB2	2.09	0.53
1:F:6:ASN:H	2:F:512:W9T:H3	1.74	0.53
1:C:415:CYS:HB3	1:C:419:THR:HG22	1.91	0.53
1:C:403:ILE:HG12	1:B:298:CYS:HB2	1.90	0.53
1:B:45:GLN:CB	1:B:57:GLU:HG3	2.39	0.53
1:D:26:GLY:H	2:D:502:W9T:H3	1.73	0.53
1:C:325:GLU:HB3	1:D:344:LYS:HB3	1.91	0.53
1:C:45:GLN:CB	1:C:57:GLU:HG3	2.39	0.53
1:C:336:PHE:HB2	1:B:334:VAL:HB	1.91	0.52
1:A:94:ARG:NH1	1:A:138:ASN:HD21	2.08	0.52
1:A:17:LYS:HG2	1:A:126:ASP:HB2	1.90	0.52
1:C:313:SER:HB3	1:C:358:SER:CB	2.39	0.52
1:E:334:VAL:HG13	1:E:335:ILE:HD12	1.91	0.52
1:A:45:GLN:CB	1:A:57:GLU:HG3	2.39	0.52
1:C:2:VAL:HG22	1:B:239:CYS:O	2.10	0.52
1:G:419:THR:HG23	1:G:429:CYS:HB3	1.92	0.52
1:A:157:ARG:NH2	1:A:183:CYS:HB3	2.25	0.52
1:F:119:CYS:O	1:F:133:VAL:HA	2.10	0.52
1:A:329:THR:HG23	1:B:340:THR:HG23	1.91	0.51
1:F:406:CYS:H	1:E:301:ASN:ND2	2.07	0.51
1:C:25:VAL:HA	2:C:1001:W9T:H2	1.91	0.51
1:B:170:GLU:HG3	2:B:502:W9T:H3	1.91	0.51
1:C:405:LYS:HA	1:B:301:ASN:HD22	1.75	0.51
1:D:313:SER:HB3	1:D:358:SER:CB	2.41	0.51
1:G:342:SER:O	1:F:326:VAL:HA	2.10	0.51
1:A:301:ASN:HB3	1:B:369:ASN:O	2.11	0.51
1:C:124:GLY:HA2	2:C:1004:W9T:C12	2.39	0.51
1:E:76:SER:HB2	1:E:77:PRO:CD	2.41	0.51
1:B:152:GLU:H	1:B:194:TYR:HD2	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:MET:HB2	1:D:382:TRP:CZ3	2.46	0.51
1:E:406:CYS:N	1:D:301:ASN:HD22	2.00	0.51
1:G:363:ILE:HD11	1:G:399:TRP:HD1	1.76	0.51
1:C:45:GLN:HB3	1:C:57:GLU:HG3	1.91	0.51
1:E:415:CYS:HB3	1:E:419:THR:HG22	1.93	0.51
1:A:76:SER:HB2	1:A:77:PRO:CD	2.41	0.51
1:C:127:GLY:HA2	5:C:1103:HOH:O	2.11	0.51
1:A:121:ASP:O	1:A:131:ILE:HA	2.10	0.51
1:B:157:ARG:NH2	1:B:183:CYS:HB3	2.26	0.51
1:A:371:ASP:OD2	1:A:405:LYS:NZ	2.44	0.51
1:D:45:GLN:CB	1:D:57:GLU:HG3	2.40	0.51
1:F:5:THR:H	2:F:512:W9T:H6	1.54	0.51
1:G:45:GLN:CB	1:G:57:GLU:HG3	2.42	0.50
1:E:363:ILE:HD11	1:E:399:TRP:CD1	2.46	0.50
1:C:296:VAL:HG22	1:D:399:TRP:CD1	2.46	0.50
1:A:45:GLN:HB3	1:A:57:GLU:HG3	1.92	0.50
1:E:125:SER:O	1:E:126:ASP:CB	2.58	0.50
1:D:76:SER:HB2	1:D:77:PRO:CD	2.40	0.50
1:A:108:ALA:HA	1:A:145:TYR:HB3	1.93	0.50
1:E:122:ILE:CG2	1:E:128:THR:O	2.59	0.50
1:G:76:SER:HB2	1:G:77:PRO:CD	2.40	0.50
1:A:334:VAL:HG13	1:A:335:ILE:HD12	1.93	0.50
1:A:336:PHE:HB2	1:G:334:VAL:HG11	1.93	0.50
1:D:45:GLN:HB3	1:D:57:GLU:HG3	1.94	0.50
1:D:371:ASP:OD2	1:D:405:LYS:NZ	2.43	0.50
1:B:14:ARG:N	1:B:145:TYR:O	2.41	0.50
1:B:419:THR:HG23	1:B:429:CYS:HB3	1.93	0.49
1:G:124:GLY:N	2:G:505:W9T:O14	2.44	0.49
1:G:371:ASP:OD2	1:G:405:LYS:NZ	2.44	0.49
1:A:118:LYS:HB3	1:A:134:TYR:N	2.26	0.49
1:F:371:ASP:OD2	1:F:405:LYS:NZ	2.43	0.49
1:E:157:ARG:NH2	1:E:183:CYS:HB3	2.27	0.49
1:G:157:ARG:NH2	1:G:183:CYS:HB3	2.27	0.49
1:A:313:SER:HB3	1:A:358:SER:CB	2.39	0.49
1:G:311:THR:OG1	1:G:360:THR:HB	2.13	0.49
1:A:372:SER:O	1:A:373:ASP:HB2	2.12	0.49
1:C:118:LYS:HB3	1:C:134:TYR:O	2.12	0.49
1:A:34:ALA:HA	1:A:131:ILE:HG13	1.93	0.49
1:C:66:ASP:OD2	1:C:74:MET:SD	2.70	0.49
1:G:25:VAL:HG23	2:G:504:W9T:H3	1.95	0.49
1:B:371:ASP:OD2	1:B:405:LYS:NZ	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:419:THR:HG23	1:F:429:CYS:HB3	1.94	0.49
1:E:134:TYR:CE1	2:E:505:W9T:H4	2.47	0.49
1:C:419:THR:HG23	1:C:429:CYS:HB3	1.90	0.49
1:B:32:ASN:ND2	1:B:72:ASN:HD21	2.11	0.49
1:F:6:ASN:HB2	2:F:512:W9T:O16	2.13	0.48
1:A:355:ASN:HB3	1:G:314:PHE:CD1	2.48	0.48
1:G:295:MET:HB2	1:G:382:TRP:CZ3	2.49	0.48
1:D:32:ASN:ND2	1:D:72:ASN:HD21	2.11	0.48
1:C:76:SER:HB2	1:C:77:PRO:CD	2.42	0.48
1:F:108:ALA:HA	1:F:145:TYR:HB3	1.96	0.48
1:E:118:LYS:HB3	1:E:134:TYR:O	2.13	0.48
1:E:32:ASN:ND2	1:E:72:ASN:HD21	2.12	0.48
1:C:2:VAL:HG13	1:B:238:TYR:CA	2.35	0.48
1:A:157:ARG:HD2	1:A:190:TRP:CH2	2.48	0.48
1:D:122:ILE:HG21	1:D:128:THR:O	2.12	0.48
1:F:157:ARG:NH2	1:F:183:CYS:HB3	2.28	0.48
1:F:32:ASN:ND2	1:F:72:ASN:HD21	2.11	0.48
1:G:45:GLN:HB3	1:G:57:GLU:HG3	1.95	0.48
1:E:326:VAL:HG12	1:E:326:VAL:O	2.13	0.48
1:B:363:ILE:HD11	1:B:399:TRP:CD1	2.49	0.48
1:A:325:GLU:HB3	1:B:344:LYS:HB3	1.96	0.48
1:G:2:VAL:HG11	1:F:278:ARG:NH1	2.29	0.48
1:B:12:GLU:O	1:B:146:VAL:HA	2.14	0.48
1:C:371:ASP:HB3	1:C:420:LYS:HG3	1.96	0.47
2:B:502:W9T:H11	2:B:502:W9T:H17	1.55	0.47
1:A:32:ASN:ND2	1:A:72:ASN:HD21	2.12	0.47
1:D:157:ARG:NH2	1:D:183:CYS:HB3	2.30	0.47
1:A:100:ASP:HB2	1:A:226:ASP:OD1	2.14	0.47
1:C:341:VAL:HA	1:B:328:SER:HA	1.97	0.47
1:F:96:LYS:HE3	1:F:140:ASP:OD1	2.14	0.47
1:D:400:ASN:HA	1:D:401:PRO:HD3	1.72	0.47
1:A:70:ASN:ND2	1:A:134:TYR:CD1	2.83	0.47
1:E:419:THR:HG23	1:E:429:CYS:HB3	1.95	0.47
1:C:371:ASP:OD2	1:C:405:LYS:NZ	2.47	0.47
1:B:214:ASP:N	1:B:214:ASP:OD1	2.44	0.47
1:C:147:ARG:HH22	1:C:198:GLU:CD	2.18	0.47
1:A:239:CYS:O	1:B:2:VAL:HG22	2.15	0.47
1:B:299:ASP:O	1:B:379:GLY:HA2	2.15	0.47
1:F:369:ASN:O	1:E:301:ASN:HB3	2.14	0.47
1:F:100:ASP:HB2	1:F:226:ASP:OD1	2.14	0.47
1:C:363:ILE:HD11	1:C:399:TRP:HD1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:371:ASP:HB3	1:F:420:LYS:HG3	1.96	0.47
1:F:363:ILE:HD11	1:F:399:TRP:CD1	2.47	0.47
1:E:34:ALA:HA	1:E:131:ILE:HG13	1.97	0.47
1:D:124:GLY:CA	2:D:506:W9T:H9	2.41	0.46
1:B:51:ASP:HB3	2:B:513:W9T:C4	2.44	0.46
1:G:123:GLU:HA	2:G:505:W9T:H2	1.96	0.46
1:E:5:THR:N	2:E:506:W9T:O14	2.49	0.46
1:C:272:ASP:HA	1:D:77:PRO:HB3	1.97	0.46
1:B:400:ASN:HA	1:B:401:PRO:HD3	1.70	0.46
1:B:17:LYS:HB2	1:B:140:ASP:O	2.16	0.46
1:A:340:THR:HG23	1:G:329:THR:HG23	1.97	0.46
1:D:311:THR:OG1	1:D:360:THR:HB	2.16	0.46
1:F:295:MET:HB2	1:F:382:TRP:CZ3	2.50	0.46
1:D:286:TRP:HB3	1:D:428:PHE:HB3	1.98	0.46
1:F:66:ASP:OD2	1:F:74:MET:SD	2.74	0.46
1:E:152:GLU:H	1:E:194:TYR:HD2	1.64	0.46
1:A:77:PRO:HB3	1:G:272:ASP:HA	1.96	0.45
1:F:76:SER:HB2	1:F:77:PRO:CD	2.45	0.45
1:D:127:GLY:HA3	1:D:128:THR:HA	1.60	0.45
1:F:152:GLU:H	1:F:194:TYR:HD2	1.64	0.45
1:F:150:GLY:HA3	1:F:195:GLU:HB3	1.98	0.45
1:G:119:CYS:O	1:G:133:VAL:HA	2.17	0.45
1:C:399:TRP:CD1	1:B:296:VAL:CG2	2.98	0.45
1:A:122:ILE:HA	1:A:130:ASP:O	2.16	0.45
1:C:123:GLU:HA	2:C:1004:W9T:H2	1.98	0.45
1:C:32:ASN:ND2	1:C:72:ASN:HD21	2.14	0.45
1:A:108:ALA:CA	1:A:145:TYR:HB3	2.45	0.45
1:G:214:ASP:N	1:G:214:ASP:OD1	2.47	0.45
1:C:418:PHE:HZ	1:B:379:GLY:HA3	1.81	0.45
1:A:94:ARG:CZ	1:A:138:ASN:HD21	2.30	0.45
1:F:121:ASP:O	1:F:131:ILE:HG23	2.17	0.45
1:C:157:ARG:HD2	1:C:190:TRP:CH2	2.52	0.45
1:D:363:ILE:HD11	1:D:399:TRP:CD1	2.50	0.45
1:F:2:VAL:HG23	1:E:238:TYR:HA	1.97	0.45
1:C:274:LEU:HD21	1:D:59:ARG:HG2	1.99	0.45
1:E:286:TRP:HB3	1:E:428:PHE:HB3	1.99	0.45
1:D:419:THR:HG23	1:D:429:CYS:HB3	1.95	0.45
1:E:96:LYS:HE3	1:E:140:ASP:OD1	2.17	0.45
1:F:400:ASN:HA	1:F:401:PRO:HD3	1.75	0.45
1:C:157:ARG:NH2	1:C:183:CYS:HB3	2.31	0.45
1:A:66:ASP:OD2	1:A:74:MET:SD	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:ASN:ND2	1:G:72:ASN:HD21	2.13	0.45
1:C:326:VAL:O	1:C:326:VAL:HG12	2.16	0.45
1:A:363:ILE:HD11	1:A:399:TRP:CD1	2.50	0.44
1:C:400:ASN:HA	1:C:401:PRO:HD3	1.72	0.44
1:A:109:THR:N	1:A:144:PHE:O	2.43	0.44
1:E:5:THR:HG1	2:E:506:W9T:H8	1.64	0.44
1:G:16:PHE:CD2	1:G:140:ASP:HB3	2.52	0.44
1:G:363:ILE:HD11	1:G:399:TRP:CD1	2.52	0.44
1:G:342:SER:HB2	1:F:327:SER:OG	2.17	0.44
1:A:2:VAL:HG13	1:G:238:TYR:CA	2.39	0.44
1:G:400:ASN:HA	1:G:401:PRO:HD3	1.72	0.44
1:G:331:GLU:HB2	1:G:340:THR:HB	2.00	0.44
1:A:2:VAL:CG1	1:G:238:TYR:HA	2.37	0.44
1:C:121:ASP:OD2	2:C:1004:W9T:H3	2.18	0.44
1:C:296:VAL:O	1:D:363:ILE:HD12	2.18	0.44
1:A:159:ARG:NH2	1:A:284:ASP:OD1	2.51	0.44
1:B:17:LYS:CD	1:B:140:ASP:HB2	2.48	0.44
1:B:295:MET:HB2	1:B:382:TRP:CZ3	2.53	0.44
1:A:286:TRP:HB3	1:A:428:PHE:HB3	2.00	0.44
1:A:419:THR:HG23	1:A:429:CYS:HB3	1.95	0.44
1:F:157:ARG:HD2	1:F:190:TRP:CH2	2.53	0.44
1:F:286:TRP:HB3	1:F:428:PHE:HB3	2.00	0.44
1:C:286:TRP:HB3	1:C:428:PHE:HB3	2.00	0.44
1:G:108:ALA:HA	1:G:144:PHE:O	2.18	0.44
1:E:6:ASN:OD1	2:E:506:W9T:H21	2.18	0.44
1:D:219:VAL:HG23	1:D:267:GLY:HA2	2.00	0.44
1:A:314:PHE:CD1	1:B:355:ASN:HB3	2.53	0.43
1:A:400:ASN:HA	1:A:401:PRO:HD3	1.73	0.43
1:B:76:SER:HB2	1:B:77:PRO:CD	2.45	0.43
1:F:311:THR:OG1	1:F:360:THR:HB	2.17	0.43
1:F:147:ARG:HH22	1:F:198:GLU:CD	2.21	0.43
1:G:66:ASP:OD2	1:G:74:MET:SD	2.76	0.43
1:G:286:TRP:HB3	1:G:428:PHE:HB3	2.00	0.43
1:D:371:ASP:HB3	1:D:420:LYS:HG3	1.99	0.43
1:C:382:TRP:O	1:C:404:VAL:HA	2.19	0.43
1:E:372:SER:OG	1:E:374:GLU:HG2	2.18	0.43
1:C:406:CYS:N	1:B:301:ASN:HD22	2.15	0.43
1:F:171:GLY:CA	2:F:503:W9T:O4	2.62	0.43
1:C:26:GLY:HA2	2:C:1001:W9T:H9	1.99	0.43
1:A:92:GLN:HG2	1:A:92:GLN:H	1.66	0.43
1:B:326:VAL:HG12	1:B:326:VAL:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LYS:HG2	1:A:126:ASP:CB	2.48	0.43
1:D:147:ARG:HH22	1:D:198:GLU:CD	2.22	0.43
1:D:231:MET:HB3	1:D:249:LYS:HD2	2.01	0.43
1:F:335:ILE:O	1:F:336:PHE:HD2	2.02	0.43
1:B:286:TRP:HB3	1:B:428:PHE:HB3	2.00	0.43
1:A:369:ASN:O	1:G:301:ASN:HB3	2.19	0.43
1:D:214:ASP:N	1:D:214:ASP:OD1	2.45	0.43
1:A:147:ARG:HH22	1:A:198:GLU:CD	2.21	0.43
1:A:127:GLY:HA3	1:A:128:THR:O	2.19	0.43
1:F:326:VAL:HG12	1:F:326:VAL:O	2.19	0.43
1:B:284:ASP:HB2	1:B:286:TRP:CD1	2.54	0.42
1:E:295:MET:HB2	1:E:382:TRP:CZ3	2.54	0.42
1:C:231:MET:HB3	1:C:249:LYS:HD2	2.00	0.42
1:C:213:SER:O	1:C:250:GLU:HG2	2.19	0.42
1:G:228:ARG:HB2	1:G:250:GLU:OE1	2.19	0.42
1:A:123:GLU:HA	2:A:1002:W9T:O14	2.19	0.42
1:F:125:SER:O	1:F:126:ASP:CB	2.64	0.42
1:C:337:ALA:CB	1:B:332:LYS:HB3	2.49	0.42
1:A:326:VAL:HG12	1:A:326:VAL:O	2.18	0.42
1:G:369:ASN:O	1:F:301:ASN:HB3	2.19	0.42
1:E:128:THR:HG22	1:E:129:GLY:H	1.84	0.42
1:G:213:SER:O	1:G:250:GLU:HG2	2.20	0.42
1:C:329:THR:HG23	1:D:340:THR:HG23	2.01	0.42
1:F:34:ALA:HA	1:F:131:ILE:HG13	2.01	0.42
1:B:92:GLN:HG2	1:B:92:GLN:H	1.66	0.42
1:G:152:GLU:H	1:G:194:TYR:HD2	1.66	0.42
1:G:231:MET:HB3	1:G:249:LYS:HD2	2.00	0.42
1:B:306:GLN:CG	1:B:381:MET:HE1	2.49	0.42
1:E:35:THR:OG1	1:E:128:THR:HG23	2.20	0.42
1:B:231:MET:HB3	1:B:249:LYS:HD2	2.02	0.42
1:A:311:THR:OG1	1:A:360:THR:HB	2.20	0.42
1:A:122:ILE:HD13	1:A:128:THR:HG22	2.02	0.42
1:G:157:ARG:HD2	1:G:190:TRP:CH2	2.55	0.42
1:D:228:ARG:HB2	1:D:250:GLU:OE1	2.19	0.42
1:E:331:GLU:HB2	1:E:340:THR:HB	2.02	0.42
1:D:25:VAL:HG23	2:D:502:W9T:C16	2.50	0.42
1:C:73:VAL:HG23	1:C:132:GLY:HA2	2.02	0.42
1:B:122:ILE:HG21	1:B:128:THR:O	2.20	0.42
1:G:16:PHE:HD2	1:G:140:ASP:HB3	1.85	0.41
1:F:284:ASP:HB2	1:F:286:TRP:CD1	2.55	0.41
1:F:214:ASP:O	1:F:251:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:THR:OG1	1:B:360:THR:HB	2.20	0.41
1:A:371:ASP:HB3	1:A:420:LYS:HG3	2.02	0.41
1:B:306:GLN:HB3	1:B:381:MET:HE2	2.02	0.41
1:A:419:THR:HG22	1:A:429:CYS:HB3	1.98	0.41
1:B:157:ARG:HD2	1:B:190:TRP:CH2	2.55	0.41
1:E:372:SER:O	1:E:373:ASP:HB2	2.20	0.41
1:E:311:THR:OG1	1:E:360:THR:HB	2.19	0.41
1:C:333:GLY:HA3	1:C:338:LYS:HG2	2.03	0.41
1:G:371:ASP:HB3	1:G:420:LYS:HG3	2.02	0.41
1:F:108:ALA:CA	1:F:145:TYR:HB3	2.50	0.41
1:E:213:SER:O	1:E:250:GLU:HG2	2.21	0.41
1:C:372:SER:O	1:C:373:ASP:HB2	2.21	0.41
1:G:333:GLY:HA2	1:G:338:LYS:HG2	2.02	0.41
1:E:122:ILE:HG21	1:E:128:THR:O	2.20	0.41
1:E:94:ARG:CZ	1:E:138:ASN:HD21	2.33	0.41
1:A:37:ASP:HB3	1:A:223:ARG:HD2	2.03	0.41
1:C:363:ILE:HD11	1:C:399:TRP:CD1	2.56	0.41
1:A:335:ILE:O	1:A:336:PHE:CD2	2.73	0.41
1:C:35:THR:HG1	1:C:129:GLY:H	1.69	0.41
1:C:228:ARG:HB2	1:C:250:GLU:OE1	2.21	0.41
1:F:59:ARG:HG2	1:E:274:LEU:HD21	2.01	0.41
1:C:243:TYR:CD2	1:C:280:LYS:HB2	2.55	0.41
1:B:331:GLU:HB2	1:B:340:THR:HB	2.03	0.41
1:D:284:ASP:HB2	1:D:286:TRP:CD1	2.55	0.41
1:A:295:MET:HB2	1:A:382:TRP:CZ3	2.56	0.41
1:D:335:ILE:O	1:D:336:PHE:CD2	2.71	0.40
1:B:219:VAL:HG23	1:B:267:GLY:HA2	2.03	0.40
1:G:335:ILE:O	1:G:336:PHE:HD2	2.04	0.40
1:F:6:ASN:N	2:F:512:W9T:H3	2.36	0.40
1:C:335:ILE:O	1:C:336:PHE:HD2	2.04	0.40
1:C:127:GLY:O	1:C:128:THR:OG1	2.36	0.40
1:B:213:SER:O	1:B:250:GLU:HG2	2.22	0.40
1:B:372:SER:O	1:B:373:ASP:HB2	2.21	0.40
1:A:333:GLY:HA3	1:A:338:LYS:HG2	2.03	0.40
1:D:331:GLU:HB2	1:D:340:THR:HB	2.02	0.40
1:B:150:GLY:HA3	1:B:195:GLU:HB3	2.02	0.40
1:G:150:GLY:HA3	1:G:195:GLU:HB3	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLY:C	3:C:1014:CA:CA[4_555]	1.19	1.01
1:A:127:GLY:CA	3:C:1014:CA:CA[4_555]	1.68	0.52
1:E:211:GLU:OE2	1:E:211:GLU:OE2[2_654]	1.69	0.51
1:B:127:GLY:O	1:D:123:GLU:OE2[4_555]	2.07	0.13

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	430/432 (100%)	407 (95%)	18 (4%)	5 (1%)	16	48
1	B	430/432 (100%)	410 (95%)	16 (4%)	4 (1%)	21	57
1	C	430/432 (100%)	410 (95%)	13 (3%)	7 (2%)	12	40
1	D	430/432 (100%)	411 (96%)	15 (4%)	4 (1%)	21	57
1	E	430/432 (100%)	408 (95%)	17 (4%)	5 (1%)	16	48
1	F	430/432 (100%)	410 (95%)	15 (4%)	5 (1%)	16	48
1	G	430/432 (100%)	411 (96%)	12 (3%)	7 (2%)	12	40
All	All	3010/3024 (100%)	2867 (95%)	106 (4%)	37 (1%)	16	48

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	ASP
1	C	128	THR
1	C	336	PHE
1	G	126	ASP
1	G	336	PHE
1	B	126	ASP
1	F	126	ASP
1	F	128	THR
1	F	336	PHE
1	E	126	ASP

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Mol	Chain	Res	Type
1	E	127	GLY
1	D	126	ASP
1	A	127	GLY
1	A	336	PHE
1	C	127	GLY
1	G	127	GLY
1	B	336	PHE
1	E	336	PHE
1	D	336	PHE
1	C	152	GLU
1	B	226	ASP
1	E	152	GLU
1	D	152	GLU
1	D	226	ASP
1	A	126	ASP
1	A	128	THR
1	C	226	ASP
1	G	152	GLU
1	G	226	ASP
1	G	333	GLY
1	B	152	GLU
1	F	152	GLU
1	A	152	GLU
1	G	335	ILE
1	E	226	ASP
1	C	335	ILE
1	F	335	ILE

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	370/370 (100%)	340 (92%)	30 (8%)	15	39
1	B	370/370 (100%)	337 (91%)	33 (9%)	12	35
1	C	370/370 (100%)	340 (92%)	30 (8%)	15	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	370/370 (100%)	337 (91%)	33 (9%)	12	35
1	E	370/370 (100%)	339 (92%)	31 (8%)	14	37
1	F	370/370 (100%)	341 (92%)	29 (8%)	16	41
1	G	370/370 (100%)	340 (92%)	30 (8%)	15	39
All	All	2590/2590 (100%)	2374 (92%)	216 (8%)	14	38

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	3	LEU
1	A	97	THR
1	A	121	ASP
1	A	125	SER
1	A	128	THR
1	A	137	GLN
1	A	167	LEU
1	A	190	TRP
1	A	209	ASP
1	A	213	SER
1	A	229	ASP
1	A	256	ASP
1	A	296	VAL
1	A	306	GLN
1	A	329	THR
1	A	334	VAL
1	A	336	PHE
1	A	340	THR
1	A	341	VAL
1	A	346	THR
1	A	360	THR
1	A	363	ILE
1	A	364	THR
1	A	384	LEU
1	A	387	GLU
1	A	396	LEU
1	A	397	LEU
1	A	411	THR
1	A	427	THR
1	C	2	VAL
1	C	3	LEU

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Mol	Chain	Res	Type
1	C	30	SER
1	C	97	THR
1	C	109	THR
1	C	121	ASP
1	C	125	SER
1	C	137	GLN
1	C	167	LEU
1	C	188	ASP
1	C	190	TRP
1	C	209	ASP
1	C	213	SER
1	C	256	ASP
1	C	296	VAL
1	C	306	GLN
1	C	322	VAL
1	C	329	THR
1	C	340	THR
1	C	346	THR
1	C	349	LEU
1	C	360	THR
1	C	363	ILE
1	C	364	THR
1	C	384	LEU
1	C	387	GLU
1	C	396	LEU
1	C	397	LEU
1	C	411	THR
1	C	427	THR
1	G	30	SER
1	G	97	THR
1	G	109	THR
1	G	121	ASP
1	G	125	SER
1	G	137	GLN
1	G	167	LEU
1	G	188	ASP
1	G	190	TRP
1	G	209	ASP
1	G	213	SER
1	G	229	ASP
1	G	256	ASP
1	G	296	VAL

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Mol	Chain	Res	Type
1	G	306	GLN
1	G	322	VAL
1	G	324	VAL
1	G	326	VAL
1	G	329	THR
1	G	340	THR
1	G	346	THR
1	G	360	THR
1	G	363	ILE
1	G	364	THR
1	G	384	LEU
1	G	387	GLU
1	G	396	LEU
1	G	397	LEU
1	G	411	THR
1	G	427	THR
1	B	2	VAL
1	B	3	LEU
1	B	30	SER
1	B	92	GLN
1	B	97	THR
1	B	121	ASP
1	B	125	SER
1	B	137	GLN
1	B	167	LEU
1	B	188	ASP
1	B	190	TRP
1	B	209	ASP
1	B	213	SER
1	B	214	ASP
1	B	229	ASP
1	B	256	ASP
1	B	296	VAL
1	B	306	GLN
1	B	329	THR
1	B	334	VAL
1	B	336	PHE
1	B	340	THR
1	B	341	VAL
1	B	346	THR
1	B	360	THR
1	B	363	ILE

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Mol	Chain	Res	Type
1	B	364	THR
1	B	384	LEU
1	B	387	GLU
1	B	396	LEU
1	B	397	LEU
1	B	411	THR
1	B	427	THR
1	F	3	LEU
1	F	30	SER
1	F	97	THR
1	F	109	THR
1	F	125	SER
1	F	128	THR
1	F	137	GLN
1	F	167	LEU
1	F	188	ASP
1	F	190	TRP
1	F	209	ASP
1	F	213	SER
1	F	229	ASP
1	F	256	ASP
1	F	296	VAL
1	F	306	GLN
1	F	329	THR
1	F	334	VAL
1	F	340	THR
1	F	346	THR
1	F	360	THR
1	F	363	ILE
1	F	364	THR
1	F	384	LEU
1	F	387	GLU
1	F	396	LEU
1	F	397	LEU
1	F	411	THR
1	F	427	THR
1	E	2	VAL
1	E	3	LEU
1	E	30	SER
1	E	97	THR
1	E	109	THR
1	E	121	ASP

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Mol	Chain	Res	Type
1	E	125	SER
1	E	128	THR
1	E	137	GLN
1	E	167	LEU
1	E	190	TRP
1	E	209	ASP
1	E	213	SER
1	E	214	ASP
1	E	256	ASP
1	E	296	VAL
1	E	306	GLN
1	E	329	THR
1	E	334	VAL
1	E	336	PHE
1	E	340	THR
1	E	346	THR
1	E	360	THR
1	E	363	ILE
1	E	364	THR
1	E	384	LEU
1	E	387	GLU
1	E	396	LEU
1	E	397	LEU
1	E	411	THR
1	E	427	THR
1	D	2	VAL
1	D	3	LEU
1	D	30	SER
1	D	92	GLN
1	D	97	THR
1	D	109	THR
1	D	120	LEU
1	D	121	ASP
1	D	125	SER
1	D	128	THR
1	D	137	GLN
1	D	167	LEU
1	D	190	TRP
1	D	209	ASP
1	D	213	SER
1	D	229	ASP
1	D	256	ASP

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Mol	Chain	Res	Type
1	D	296	VAL
1	D	306	GLN
1	D	326	VAL
1	D	329	THR
1	D	336	PHE
1	D	340	THR
1	D	346	THR
1	D	360	THR
1	D	363	ILE
1	D	364	THR
1	D	384	LEU
1	D	387	GLU
1	D	396	LEU
1	D	397	LEU
1	D	411	THR
1	D	427	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	270	GLN
1	A	301	ASN
1	A	306	GLN
1	C	32	ASN
1	C	270	GLN
1	C	301	ASN
1	C	306	GLN
1	G	32	ASN
1	G	301	ASN
1	G	306	GLN
1	B	32	ASN
1	B	301	ASN
1	B	306	GLN
1	F	32	ASN
1	F	138	ASN
1	F	270	GLN
1	F	301	ASN
1	F	306	GLN
1	E	32	ASN
1	E	138	ASN
1	E	270	GLN

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Mol	Chain	Res	Type
1	E	301	ASN
1	E	306	GLN
1	D	32	ASN
1	D	270	GLN
1	D	301	ASN
1	D	306	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	A	1	1	7,8,9	0.52	0	9,10,12	2.24	2 (22%)
1	PCA	B	1	1	7,8,9	0.46	0	9,10,12	2.11	2 (22%)
1	PCA	C	1	1	7,8,9	0.48	0	9,10,12	2.22	2 (22%)
1	PCA	D	1	1	7,8,9	0.58	0	9,10,12	2.21	2 (22%)
1	PCA	E	1	1	7,8,9	0.42	0	9,10,12	2.30	2 (22%)
1	PCA	F	1	1	7,8,9	0.46	0	9,10,12	2.16	2 (22%)
1	PCA	G	1	1	7,8,9	0.60	0	9,10,12	2.10	2 (22%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1
1	PCA	F	1	1	-	0/0/11/13	0/1/1/1
1	PCA	G	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1	PCA	CA-N-CD	-4.48	98.79	113.81
1	A	1	PCA	CA-N-CD	-4.09	100.12	113.81
1	C	1	PCA	CA-N-CD	-3.88	100.80	113.81
1	E	1	PCA	CA-N-CD	-3.88	100.81	113.81
1	B	1	PCA	CA-N-CD	-3.81	101.05	113.81
1	G	1	PCA	CA-N-CD	-3.77	101.19	113.81
1	D	1	PCA	CA-N-CD	-3.63	101.65	113.81
1	F	1	PCA	CB-CA-C	3.36	117.36	112.76
1	G	1	PCA	CB-CA-C	4.11	118.38	112.76
1	B	1	PCA	CB-CA-C	4.23	118.55	112.76
1	A	1	PCA	CB-CA-C	4.34	118.70	112.76
1	C	1	PCA	CB-CA-C	4.46	118.87	112.76
1	E	1	PCA	CB-CA-C	4.89	119.45	112.76
1	D	1	PCA	CB-CA-C	4.99	119.59	112.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 58 are monoatomic - leaving 37 for Mogul analysis.

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	W9T	A	1001	3	23,24,24	0.58	0	28,36,36	1.21	2 (7%)
2	W9T	A	1002	3	23,24,24	0.67	0	28,36,36	1.30	3 (10%)
2	W9T	A	1003	3	23,24,24	0.51	0	28,36,36	0.86	2 (7%)
2	W9T	A	1004	3	23,24,24	0.59	1 (4%)	28,36,36	0.95	0
2	W9T	A	1012	3	23,24,24	0.50	0	28,36,36	0.90	0
2	W9T	B	501	3	23,24,24	0.61	0	28,36,36	1.18	2 (7%)
2	W9T	B	502	3	23,24,24	0.73	0	28,36,36	1.46	4 (14%)
2	W9T	B	503	3	23,24,24	0.54	0	28,36,36	0.90	1 (3%)
2	W9T	B	504	3	23,24,24	0.60	0	28,36,36	1.73	6 (21%)
2	W9T	B	507	3	23,24,24	0.54	0	28,36,36	1.41	2 (7%)
2	W9T	B	513	-	23,24,24	0.83	1 (4%)	28,36,36	2.17	6 (21%)
2	W9T	C	1001	3	23,24,24	0.77	0	28,36,36	1.45	3 (10%)
2	W9T	C	1002	3	23,24,24	0.53	0	28,36,36	1.17	2 (7%)
2	W9T	C	1003	3	23,24,24	0.59	0	28,36,36	1.23	2 (7%)
2	W9T	C	1004	3	23,24,24	0.60	0	28,36,36	1.47	5 (17%)
2	W9T	C	1005	3	23,24,24	0.65	0	28,36,36	0.84	1 (3%)
2	W9T	D	501	3	23,24,24	0.60	1 (4%)	28,36,36	1.05	1 (3%)
2	W9T	D	502	3	23,24,24	0.60	0	28,36,36	1.15	2 (7%)
2	W9T	D	506	3	23,24,24	0.59	0	28,36,36	0.98	0
2	W9T	D	507	3	23,24,24	0.59	0	28,36,36	1.43	4 (14%)
2	W9T	D	512	3	23,24,24	0.45	0	28,36,36	1.24	3 (10%)
2	W9T	E	501	3	23,24,24	0.63	0	28,36,36	1.27	2 (7%)
2	W9T	E	502	3	23,24,24	0.58	0	28,36,36	1.13	2 (7%)
2	W9T	E	503	3	23,24,24	0.61	1 (4%)	28,36,36	1.09	3 (10%)
2	W9T	E	504	3	23,24,24	0.63	0	28,36,36	1.04	1 (3%)
2	W9T	E	505	3	23,24,24	0.63	0	28,36,36	1.24	4 (14%)
2	W9T	E	506	-	23,24,24	0.61	0	28,36,36	1.64	6 (21%)
2	W9T	F	501	3	23,24,24	0.64	0	28,36,36	0.94	1 (3%)
2	W9T	F	502	3	23,24,24	0.60	0	28,36,36	0.78	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	W9T	F	503	3	23,24,24	0.81	1 (4%)	28,36,36	1.61	5 (17%)
2	W9T	F	504	3	23,24,24	0.57	0	28,36,36	0.98	2 (7%)
2	W9T	F	512	-	23,24,24	0.80	0	28,36,36	1.82	9 (32%)
2	W9T	G	501	3	23,24,24	0.55	0	28,36,36	0.89	2 (7%)
2	W9T	G	502	3	23,24,24	0.59	0	28,36,36	0.94	1 (3%)
2	W9T	G	503	3	23,24,24	0.55	0	28,36,36	1.49	4 (14%)
2	W9T	G	504	3	23,24,24	0.53	0	28,36,36	0.93	1 (3%)
2	W9T	G	505	3	23,24,24	0.56	0	28,36,36	1.28	3 (10%)

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	W9T	A	1001	3	-	0/11/50/50	0/2/2/2
2	W9T	A	1002	3	-	0/11/50/50	0/2/2/2
2	W9T	A	1003	3	-	0/11/50/50	0/2/2/2
2	W9T	A	1004	3	-	0/11/50/50	0/2/2/2
2	W9T	A	1012	3	-	0/11/50/50	0/2/2/2
2	W9T	B	501	3	-	0/11/50/50	0/2/2/2
2	W9T	B	502	3	-	0/11/50/50	0/2/2/2
2	W9T	B	503	3	-	0/11/50/50	0/2/2/2
2	W9T	B	504	3	-	0/11/50/50	0/2/2/2
2	W9T	B	507	3	-	0/11/50/50	0/2/2/2
2	W9T	B	513	-	-	0/11/50/50	0/2/2/2
2	W9T	C	1001	3	-	0/11/50/50	0/2/2/2
2	W9T	C	1002	3	-	0/11/50/50	0/2/2/2
2	W9T	C	1003	3	-	0/11/50/50	0/2/2/2
2	W9T	C	1004	3	-	0/11/50/50	0/2/2/2
2	W9T	C	1005	3	-	0/11/50/50	0/2/2/2
2	W9T	D	501	3	-	0/11/50/50	0/2/2/2
2	W9T	D	502	3	-	0/11/50/50	0/2/2/2
2	W9T	D	506	3	-	0/11/50/50	0/2/2/2
2	W9T	D	507	3	-	0/11/50/50	0/2/2/2
2	W9T	D	512	3	-	0/11/50/50	0/2/2/2
2	W9T	E	501	3	-	0/11/50/50	0/2/2/2
2	W9T	E	502	3	-	0/11/50/50	0/2/2/2
2	W9T	E	503	3	-	0/11/50/50	0/2/2/2
2	W9T	E	504	3	-	0/11/50/50	0/2/2/2
2	W9T	E	505	3	-	0/11/50/50	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	W9T	E	506	-	-	0/11/50/50	0/2/2/2
2	W9T	F	501	3	-	0/11/50/50	0/2/2/2
2	W9T	F	502	3	-	0/11/50/50	0/2/2/2
2	W9T	F	503	3	-	0/11/50/50	0/2/2/2
2	W9T	F	504	3	-	0/11/50/50	0/2/2/2
2	W9T	F	512	-	-	0/11/50/50	0/2/2/2
2	W9T	G	501	3	-	0/11/50/50	0/2/2/2
2	W9T	G	502	3	-	0/11/50/50	0/2/2/2
2	W9T	G	503	3	-	0/11/50/50	0/2/2/2
2	W9T	G	504	3	-	0/11/50/50	0/2/2/2
2	W9T	G	505	3	-	0/11/50/50	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	W9T	O2-C2	2.00	1.44	1.41
2	B	513	W9T	O2-C2	2.02	1.44	1.41
2	A	1004	W9T	O2-C2	2.02	1.44	1.41
2	E	503	W9T	O2-C2	2.05	1.44	1.41
2	F	503	W9T	O2-C2	2.06	1.44	1.41

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	513	W9T	C11-O15-C15	-7.51	99.17	113.75
2	E	506	W9T	O13-C13-C12	-4.14	101.03	110.34
2	C	1003	W9T	C11-O4-C4	-3.94	107.71	118.01
2	F	503	W9T	O4-C11-O15	-3.78	101.11	110.68
2	B	507	W9T	C11-O4-C4	-3.64	108.50	118.01
2	E	501	W9T	C11-O4-C4	-3.50	108.86	118.01
2	D	501	W9T	C11-O4-C4	-3.42	109.07	118.01
2	F	512	W9T	O15-C15-C14	-3.40	103.29	109.68
2	F	512	W9T	C11-O4-C4	-3.34	109.28	118.01
2	F	512	W9T	O4-C11-O15	-3.22	102.53	110.68
2	F	512	W9T	O13-C13-C12	-3.07	103.42	110.34
2	B	501	W9T	O4-C4-C3	-3.06	103.16	114.94
2	E	506	W9T	C11-C12-C13	-3.02	104.02	109.97
2	A	1001	W9T	C11-O4-C4	-3.01	110.15	118.01
2	E	506	W9T	O15-C15-C14	-2.98	104.08	109.68
2	B	513	W9T	O15-C15-C14	-2.93	104.17	109.68
2	G	503	W9T	C11-O4-C4	-2.90	110.44	118.01
2	B	503	W9T	C11-O4-C4	-2.83	110.60	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	512	W9T	C11-O15-C15	-2.78	108.34	113.75
2	F	512	W9T	C11-C12-C13	-2.70	104.65	109.97
2	G	501	W9T	C11-O4-C4	-2.68	111.01	118.01
2	D	512	W9T	C13-C14-C15	-2.62	105.63	110.20
2	E	503	W9T	O13-C13-C14	-2.58	104.53	110.34
2	D	507	W9T	C11-O4-C4	-2.55	111.33	118.01
2	B	501	W9T	O4-C11-C12	-2.50	102.02	108.10
2	C	1002	W9T	C13-C14-C15	-2.45	105.92	110.20
2	F	512	W9T	O4-C11-C12	-2.33	102.44	108.10
2	B	513	W9T	O13-C13-C14	-2.32	105.10	110.34
2	D	502	W9T	O4-C4-C3	-2.32	106.01	114.94
2	G	502	W9T	C11-O4-C4	-2.21	112.24	118.01
2	C	1003	W9T	O12-C12-C11	-2.18	105.25	110.02
2	E	502	W9T	C11-O4-C4	-2.14	112.43	118.01
2	A	1003	W9T	C11-O4-C4	-2.12	112.45	118.01
2	C	1004	W9T	C11-O4-C4	-2.11	112.50	118.01
2	F	512	W9T	O14-C14-C13	-2.09	105.63	110.34
2	E	505	W9T	C11-O4-C4	-2.05	112.65	118.01
2	F	502	W9T	C11-O4-C4	-2.02	112.74	118.01
2	G	504	W9T	C11-O4-C4	-2.00	112.77	118.01
2	F	504	W9T	C11-O4-C4	-2.00	112.78	118.01
2	E	506	W9T	C11-O4-C4	-2.00	112.78	118.01
2	B	504	W9T	O15-C11-C12	2.04	114.46	110.28
2	C	1004	W9T	O5-C5-C4	2.05	107.00	103.52
2	F	503	W9T	O4-C11-C12	2.06	113.12	108.10
2	A	1003	W9T	O5-C5-C4	2.06	107.01	103.52
2	G	503	W9T	O5-C5-C4	2.13	107.12	103.52
2	G	501	W9T	O5-C5-C4	2.15	107.16	103.52
2	E	503	W9T	O15-C15-C16	2.15	111.80	106.36
2	C	1001	W9T	C11-O15-C15	2.16	117.93	113.75
2	G	505	W9T	O15-C15-C14	2.17	113.76	109.68
2	B	504	W9T	O15-C15-C14	2.19	113.80	109.68
2	G	505	W9T	O5-C5-C4	2.22	107.28	103.52
2	D	507	W9T	O15-C15-C14	2.23	113.87	109.68
2	C	1002	W9T	O14-C14-C15	2.25	115.19	109.24
2	A	1002	W9T	O15-C15-C14	2.25	113.90	109.68
2	D	512	W9T	O15-C15-C16	2.25	112.04	106.36
2	C	1005	W9T	O5-C5-C4	2.27	107.36	103.52
2	F	503	W9T	C11-O15-C15	2.30	118.22	113.75
2	E	503	W9T	O5-C5-C4	2.32	107.44	103.52
2	D	507	W9T	O5-C5-C4	2.35	107.50	103.52
2	F	504	W9T	C13-C14-C15	2.38	114.34	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	512	W9T	O15-C15-C16	2.39	112.39	106.36
2	E	506	W9T	O5-C5-C4	2.40	107.57	103.52
2	E	501	W9T	O15-C11-C12	2.40	115.20	110.28
2	E	502	W9T	O5-C5-C4	2.43	107.62	103.52
2	B	502	W9T	O5-C5-C4	2.45	107.66	103.52
2	E	505	W9T	O5-C5-C4	2.47	107.70	103.52
2	D	512	W9T	O5-C5-C4	2.58	107.89	103.52
2	E	504	W9T	O15-C15-C16	2.59	112.90	106.36
2	E	506	W9T	O15-C15-C16	2.67	113.10	106.36
2	A	1002	W9T	O5-C5-C4	2.70	108.08	103.52
2	A	1001	W9T	O15-C15-C16	2.72	113.23	106.36
2	F	501	W9T	O5-C5-C4	2.73	108.14	103.52
2	B	502	W9T	C11-O15-C15	2.75	119.09	113.75
2	B	504	W9T	C11-C12-C13	2.77	115.44	109.97
2	D	502	W9T	C11-O15-C15	2.83	119.23	113.75
2	B	502	W9T	O14-C14-C15	2.89	116.90	109.24
2	E	505	W9T	O15-C15-C16	2.90	113.69	106.36
2	E	505	W9T	C11-O15-C15	2.92	119.41	113.75
2	C	1004	W9T	C11-O15-C15	3.00	119.57	113.75
2	B	513	W9T	C11-O4-C4	3.01	125.86	118.01
2	B	513	W9T	O15-C15-C16	3.02	113.98	106.36
2	C	1004	W9T	C13-C14-C15	3.15	115.69	110.20
2	G	503	W9T	O15-C15-C14	3.24	115.76	109.68
2	B	502	W9T	O15-C15-C14	3.26	115.80	109.68
2	G	505	W9T	C11-O15-C15	3.31	120.17	113.75
2	F	503	W9T	C11-C12-C13	3.31	116.50	109.97
2	B	504	W9T	C11-O15-C15	3.40	120.34	113.75
2	B	507	W9T	C11-O15-C15	3.44	120.43	113.75
2	C	1001	W9T	O15-C15-C14	3.54	116.33	109.68
2	A	1002	W9T	C11-O15-C15	3.66	120.85	113.75
2	F	503	W9T	C11-O4-C4	3.69	127.66	118.01
2	G	503	W9T	C11-O15-C15	3.77	121.06	113.75
2	B	513	W9T	O4-C11-O15	3.80	120.30	110.68
2	B	504	W9T	C13-C14-C15	4.04	117.23	110.20
2	B	504	W9T	C14-C13-C12	4.14	118.51	110.79
2	D	507	W9T	C11-O15-C15	4.51	122.50	113.75
2	C	1004	W9T	O15-C15-C14	4.75	118.61	109.68
2	C	1001	W9T	C13-C14-C15	4.82	118.60	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	W9T	3	0
2	B	502	W9T	2	0
2	B	504	W9T	2	0
2	B	513	W9T	2	0
2	C	1001	W9T	2	0
2	C	1004	W9T	6	0
2	D	502	W9T	2	0
2	D	506	W9T	2	0
2	E	505	W9T	3	0
2	E	506	W9T	8	0
2	F	503	W9T	3	0
2	F	512	W9T	5	0
2	G	504	W9T	1	0
2	G	505	W9T	4	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	431/432 (99%)	0.60	31 (7%) 18 12	42, 73, 121, 211	0
1	B	431/432 (99%)	0.52	31 (7%) 18 12	44, 73, 111, 196	0
1	C	431/432 (99%)	0.50	28 (6%) 22 16	47, 75, 114, 165	0
1	D	431/432 (99%)	0.48	31 (7%) 18 12	43, 77, 119, 218	0
1	E	431/432 (99%)	0.60	35 (8%) 15 9	45, 73, 123, 193	0
1	F	431/432 (99%)	0.68	43 (9%) 9 5	46, 74, 137, 209	0
1	G	431/432 (99%)	0.84	47 (10%) 7 4	43, 77, 138, 211	0
All	All	3017/3024 (99%)	0.60	246 (8%) 14 9	42, 75, 124, 218	0

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	334	VAL	12.9
1	G	337	ALA	12.0
1	E	335	ILE	11.6
1	G	334	VAL	11.3
1	G	333	GLY	10.6
1	E	333	GLY	9.8
1	B	336	PHE	9.0
1	G	125	SER	8.4
1	A	334	VAL	7.9
1	G	330	ILE	7.9
1	A	333	GLY	7.8
1	A	335	ILE	7.8
1	G	336	PHE	7.5
1	D	335	ILE	7.3
1	A	336	PHE	7.1
1	A	331	GLU	7.1
1	F	334	VAL	7.1

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Mol	Chain	Res	Type	RSRZ
1	D	333	GLY	7.0
1	B	335	ILE	6.9
1	D	226	ASP	6.7
1	D	337	ALA	6.7
1	F	134	TYR	6.6
1	E	136	CYS	6.5
1	A	133	VAL	6.4
1	G	335	ILE	6.4
1	E	332	LYS	6.3
1	D	334	VAL	6.3
1	F	333	GLY	6.3
1	C	335	ILE	6.3
1	E	338	LYS	6.1
1	E	339	ALA	5.9
1	A	134	TYR	5.7
1	B	337	ALA	5.7
1	G	339	ALA	5.7
1	G	328	SER	5.7
1	G	338	LYS	5.6
1	E	336	PHE	5.6
1	A	337	ALA	5.6
1	A	338	LYS	5.5
1	G	332	LYS	5.4
1	B	333	GLY	5.4
1	D	336	PHE	5.4
1	B	139	LEU	5.2
1	B	338	LYS	5.0
1	F	335	ILE	5.0
1	F	133	VAL	5.0
1	F	337	ALA	4.9
1	G	140	ASP	4.7
1	F	336	PHE	4.7
1	G	141	ASP	4.6
1	B	228	ARG	4.6
1	A	68	SER	4.6
1	A	142	GLN	4.5
1	E	331	GLU	4.4
1	C	333	GLY	4.4
1	E	125	SER	4.4
1	F	338	LYS	4.3
1	E	337	ALA	4.2
1	B	334	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	334	VAL	4.1
1	B	332	LYS	4.1
1	A	136	CYS	4.1
1	E	142	GLN	4.0
1	G	123	GLU	4.0
1	C	134	TYR	4.0
1	G	341	VAL	4.0
1	G	222	TYR	4.0
1	G	135	ASP	4.0
1	D	331	GLU	4.0
1	F	142	GLN	4.0
1	E	123	GLU	4.0
1	A	325	GLU	3.9
1	A	122	ILE	3.9
1	G	326	VAL	3.8
1	G	343	VAL	3.8
1	G	340	THR	3.8
1	D	338	LYS	3.8
1	G	331	GLU	3.8
1	C	222	TYR	3.8
1	F	94	ARG	3.8
1	G	142	GLN	3.8
1	D	137	GLN	3.7
1	A	70	ASN	3.7
1	C	327	SER	3.7
1	G	136	CYS	3.6
1	G	342	SER	3.6
1	E	68	SER	3.6
1	D	213	SER	3.6
1	G	122	ILE	3.5
1	C	340	THR	3.5
1	F	211	GLU	3.5
1	D	339	ALA	3.5
1	F	342	SER	3.5
1	A	67	GLY	3.5
1	E	325	GLU	3.5
1	F	314	PHE	3.5
1	F	332	LYS	3.5
1	F	331	GLU	3.5
1	A	339	ALA	3.5
1	B	339	ALA	3.5
1	D	139	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	329	THR	3.4
1	F	389	THR	3.4
1	B	224	CYS	3.4
1	F	330	ILE	3.4
1	G	134	TYR	3.3
1	F	136	CYS	3.2
1	G	237	ALA	3.2
1	E	69	GLY	3.2
1	F	341	VAL	3.2
1	D	136	CYS	3.2
1	E	342	SER	3.1
1	C	331	GLU	3.1
1	B	222	TYR	3.1
1	E	134	TYR	3.1
1	B	216	SER	3.1
1	E	226	ASP	3.1
1	D	228	ARG	3.0
1	F	17	LYS	3.0
1	C	125	SER	3.0
1	B	331	GLU	3.0
1	D	227	LEU	3.0
1	C	336	PHE	3.0
1	B	314	PHE	3.0
1	G	133	VAL	3.0
1	F	69	GLY	3.0
1	E	141	ASP	3.0
1	B	364	THR	2.9
1	F	364	THR	2.9
1	B	143	TYR	2.9
1	F	141	ASP	2.9
1	G	211	GLU	2.9
1	C	127	GLY	2.9
1	B	135	ASP	2.9
1	D	342	SER	2.9
1	A	138	ASN	2.9
1	D	122	ILE	2.9
1	E	137	GLN	2.9
1	F	68	SER	2.8
1	F	328	SER	2.8
1	B	217	GLY	2.8
1	G	118	LYS	2.8
1	D	250	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	325	GLU	2.8
1	F	339	ALA	2.8
1	G	224	CYS	2.7
1	E	314	PHE	2.7
1	F	329	THR	2.7
1	F	388	THR	2.7
1	D	327	SER	2.7
1	C	169	VAL	2.7
1	C	211	GLU	2.7
1	E	122	ILE	2.7
1	B	141	ASP	2.7
1	G	215	GLY	2.7
1	D	66	ASP	2.7
1	A	342	SER	2.7
1	B	213	SER	2.7
1	E	140	ASP	2.6
1	B	133	VAL	2.6
1	C	170	GLU	2.6
1	E	139	LEU	2.6
1	D	125	SER	2.6
1	G	71	ALA	2.6
1	G	210	VAL	2.6
1	C	424	GLU	2.5
1	G	247	LEU	2.5
1	G	36	TYR	2.5
1	C	329	THR	2.5
1	D	332	LYS	2.5
1	G	128	THR	2.5
1	E	364	THR	2.5
1	C	325	GLU	2.5
1	F	135	ASP	2.5
1	E	215	GLY	2.5
1	C	307	GLN	2.4
1	F	125	SER	2.4
1	F	128	THR	2.4
1	F	122	ILE	2.4
1	C	126	ASP	2.4
1	C	346	THR	2.4
1	F	325	GLU	2.4
1	C	339	ALA	2.4
1	A	364	THR	2.4
1	F	183	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	69	GLY	2.4
1	C	68	SER	2.4
1	C	328	SER	2.4
1	G	226	ASP	2.4
1	A	330	ILE	2.4
1	F	123	GLU	2.4
1	A	135	ASP	2.4
1	D	224	CYS	2.3
1	E	340	THR	2.3
1	A	115	ALA	2.3
1	A	332	LYS	2.3
1	G	387	GLU	2.3
1	A	128	THR	2.3
1	B	340	THR	2.3
1	G	16	PHE	2.3
1	D	141	ASP	2.3
1	F	353	TRP	2.3
1	B	215	GLY	2.3
1	F	67	GLY	2.3
1	E	29	GLY	2.3
1	C	143	TYR	2.3
1	D	133	VAL	2.3
1	E	143	TYR	2.2
1	A	143	TYR	2.2
1	F	320	ALA	2.2
1	G	227	LEU	2.2
1	B	325	GLU	2.2
1	E	138	ASN	2.2
1	C	139	LEU	2.2
1	G	324	VAL	2.2
1	C	347	ALA	2.2
1	D	128	THR	2.2
1	D	222	TYR	2.2
1	G	17	LYS	2.1
1	F	355	ASN	2.1
1	G	121	ASP	2.1
1	E	424	GLU	2.1
1	G	65	PRO	2.1
1	F	324	VAL	2.1
1	E	133	VAL	2.1
1	B	123	GLU	2.1
1	B	170	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	131	ILE	2.1
1	B	307	GLN	2.1
1	B	134	TYR	2.1
1	F	186	ASN	2.1
1	D	143	TYR	2.1
1	D	147	ARG	2.1
1	C	128	THR	2.1
1	A	125	SER	2.1
1	A	428	PHE	2.1
1	D	314	PHE	2.1
1	B	140	ASP	2.0
1	F	118	LYS	2.0
1	G	119	CYS	2.0
1	E	307	GLN	2.0
1	G	139	LEU	2.0
1	C	342	SER	2.0
1	B	305	SER	2.0
1	E	344	LYS	2.0
1	F	343	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PCA	F	1	8/9	0.82	0.25	-	65,67,70,72	0
1	PCA	G	1	8/9	0.93	0.24	-	74,76,80,81	0
1	PCA	E	1	8/9	0.84	0.27	-	86,95,99,101	0
1	PCA	C	1	8/9	0.86	0.31	-	76,88,94,96	0
1	PCA	A	1	8/9	0.84	0.24	-	83,87,93,93	0
1	PCA	B	1	8/9	0.93	0.24	-	68,77,80,82	0
1	PCA	D	1	8/9	0.88	0.23	-	76,82,87,88	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	W9T	F	512	23/23	0.91	0.26	1.74	68,78,85,91	0
2	W9T	B	513	23/23	0.93	0.24	1.05	61,70,76,86	0
2	W9T	E	506	23/23	0.94	0.24	0.69	78,85,94,102	0
2	W9T	B	501	23/23	0.93	0.22	0.45	79,86,115,120	0
2	W9T	F	503	23/23	0.84	0.27	0.18	85,100,105,112	0
2	W9T	B	503	23/23	0.90	0.21	0.10	94,105,118,121	0
2	W9T	D	502	23/23	0.86	0.24	0.09	109,121,134,139	0
2	W9T	C	1004	23/23	0.86	0.30	0.06	100,120,137,138	0
3	CA	C	1008	1/1	0.93	0.19	0.03	69,69,69,69	0
2	W9T	G	505	23/23	0.81	0.42	0.02	140,157,166,168	0
2	W9T	E	505	23/23	0.78	0.40	0.00	132,151,158,161	0
3	CA	D	508	1/1	0.93	0.19	-0.05	80,80,80,80	0
3	CA	F	505	1/1	0.96	0.19	-0.21	61,61,61,61	0
2	W9T	D	501	23/23	0.92	0.19	-0.30	75,86,102,104	0
2	W9T	A	1012	23/23	0.92	0.18	-0.37	72,79,105,116	0
2	W9T	C	1002	23/23	0.90	0.25	-0.42	73,83,117,119	0
2	W9T	A	1004	23/23	0.94	0.20	-0.48	67,80,103,121	0
2	W9T	B	504	23/23	0.85	0.25	-0.48	92,116,139,148	0
2	W9T	E	503	23/23	0.91	0.19	-0.49	58,74,104,107	0
2	W9T	E	504	23/23	0.90	0.18	-0.53	79,86,120,123	0
2	W9T	B	502	23/23	0.92	0.23	-0.56	69,81,98,105	0
2	W9T	F	501	23/23	0.93	0.16	-0.58	69,78,101,102	0
3	CA	C	1006	1/1	0.97	0.18	-0.59	65,65,65,65	0
2	W9T	D	512	23/23	0.92	0.18	-0.60	75,89,106,108	0
3	CA	D	505	1/1	0.97	0.17	-0.63	68,68,68,68	0
4	MG	E	512	1/1	0.97	0.16	-0.68	54,54,54,54	0
3	CA	C	1014	1/1	0.97	0.21	-0.71	60,60,60,60	0
2	W9T	A	1002	23/23	0.80	0.23	-0.72	100,117,129,132	0
3	CA	B	508	1/1	0.98	0.17	-0.75	79,79,79,79	0
2	W9T	C	1003	23/23	0.94	0.18	-0.75	74,89,117,130	0
3	CA	A	1008	1/1	0.98	0.16	-0.78	66,66,66,66	0
3	CA	A	1005	1/1	0.98	0.16	-0.78	70,70,70,70	0
2	W9T	F	502	23/23	0.94	0.19	-0.79	74,82,99,101	0
3	CA	F	507	1/1	0.99	0.15	-0.82	76,76,76,76	0
2	W9T	E	501	23/23	0.96	0.16	-0.83	59,67,80,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	W9T	E	502	23/23	0.91	0.20	-0.84	65,82,101,103	0
3	CA	E	509	1/1	0.97	0.15	-0.87	65,65,65,65	0
2	W9T	C	1001	23/23	0.85	0.16	-0.91	85,103,132,143	0
2	W9T	F	504	23/23	0.87	0.20	-0.92	90,101,105,109	0
2	W9T	D	507	23/23	0.91	0.18	-1.05	69,90,112,121	0
2	W9T	C	1005	23/23	0.83	0.17	-1.08	96,114,124,125	0
3	CA	F	508	1/1	0.91	0.18	-1.09	70,70,70,70	0
2	W9T	G	502	23/23	0.93	0.16	-1.11	63,72,99,106	0
3	CA	A	1009	1/1	0.98	0.18	-1.11	68,68,68,68	0
2	W9T	G	503	23/23	0.90	0.21	-1.18	86,101,126,130	0
2	W9T	A	1003	23/23	0.92	0.18	-1.19	73,87,119,125	0
3	CA	C	1010	1/1	0.91	0.14	-1.19	91,91,91,91	0
3	CA	E	508	1/1	0.98	0.16	-1.21	55,55,55,55	0
3	CA	G	509	1/1	0.96	0.15	-1.21	66,66,66,66	0
2	W9T	B	507	23/23	0.93	0.16	-1.32	70,96,115,121	0
2	W9T	D	506	23/23	0.91	0.18	-1.34	98,111,133,137	0
2	W9T	A	1001	23/23	0.94	0.14	-1.50	79,83,98,100	0
2	W9T	G	504	23/23	0.91	0.14	-1.51	92,96,110,112	0
3	CA	B	505	1/1	0.95	0.13	-1.51	64,64,64,64	0
3	CA	E	510	1/1	0.97	0.11	-1.66	95,95,95,95	0
3	CA	G	508	1/1	0.88	0.12	-1.73	84,84,84,84	0
4	MG	D	510	1/1	0.86	0.10	-1.74	85,85,85,85	0
3	CA	C	1007	1/1	0.88	0.12	-1.81	64,64,64,64	0
3	CA	B	506	1/1	0.97	0.14	-1.84	75,75,75,75	0
4	MG	B	512	1/1	0.92	0.07	-1.91	70,70,70,70	0
3	CA	C	1009	1/1	0.96	0.11	-1.97	75,75,75,75	0
3	CA	A	1007	1/1	0.96	0.12	-1.98	67,67,67,67	0
4	MG	G	511	1/1	0.99	0.09	-2.02	74,74,74,74	0
3	CA	B	510	1/1	0.94	0.11	-2.04	85,85,85,85	0
3	CA	A	1006	1/1	0.94	0.09	-2.09	92,92,92,92	0
4	MG	D	511	1/1	0.96	0.11	-2.11	83,83,83,83	0
3	CA	G	510	1/1	0.98	0.09	-2.13	83,83,83,83	0
4	MG	A	1011	1/1	0.88	0.08	-2.15	72,72,72,72	0
3	CA	B	509	1/1	0.96	0.08	-2.16	96,96,96,96	0
3	CA	D	504	1/1	0.98	0.05	-2.18	84,84,84,84	0
4	MG	A	1010	1/1	0.90	0.12	-2.20	59,59,59,59	0
3	CA	D	503	1/1	0.91	0.11	-2.21	73,73,73,73	0
2	W9T	G	501	23/23	0.95	0.14	-2.24	85,95,99,104	0
4	MG	E	513	1/1	0.69	0.12	-2.29	109,109,109,109	0
3	CA	G	506	1/1	0.94	0.06	-2.29	116,116,116,116	0
4	MG	C	1011	1/1	0.95	0.05	-2.34	86,86,86,86	0
3	CA	F	506	1/1	0.98	0.14	-2.39	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	F	509	1/1	0.94	0.10	-2.42	53,53,53,53	0
3	CA	E	507	1/1	0.97	0.12	-2.53	60,60,60,60	0
3	CA	D	509	1/1	0.96	0.07	-2.83	97,97,97,97	0
3	CA	F	511	1/1	0.85	0.06	-2.86	127,127,127,127	0
3	CA	G	507	1/1	0.98	0.11	-2.97	72,72,72,72	0
4	MG	G	512	1/1	0.95	0.10	-3.05	108,108,108,108	0
4	MG	F	510	1/1	0.91	0.10	-3.21	68,68,68,68	0
3	CA	E	511	1/1	0.94	0.10	-3.26	123,123,123,123	0
4	MG	B	511	1/1	0.96	0.09	-3.60	84,84,84,84	0
4	MG	C	1012	1/1	0.96	0.07	-3.75	67,67,67,67	0
3	CA	C	1013	1/1	0.91	0.10	-	94,94,94,94	0
3	CA	B	514	1/1	0.92	0.06	-	88,88,88,88	0
3	CA	G	513	1/1	0.84	0.05	-	87,87,87,87	0
3	CA	E	514	1/1	0.84	0.10	-	88,88,88,88	0
3	CA	E	515	1/1	0.99	0.23	-	37,37,37,37	1
3	CA	A	1013	1/1	0.76	0.06	-	96,96,96,96	0
3	CA	D	513	1/1	0.91	0.04	-	93,93,93,93	0
3	CA	F	513	1/1	0.95	0.07	-	93,93,93,93	0

6.5 Other polymers

There are no such residues in this entry.