



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 PM GMT

PDB ID : 4M3C  
Title : Structure of a binary complex between homologous tetrameric legume lectins from *Butea monosperma* and *Spatholobus parviflorus* seeds  
Authors : Surya, S.; Abhilash, J.; Geethanandan, K.; Sadasivan, C.; Haridas, M.  
Deposited on : 2013-08-06  
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](mailto: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.

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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

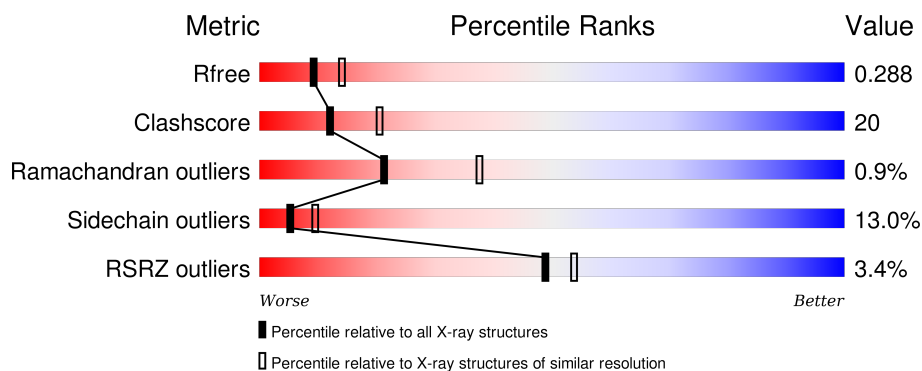
# 1 Overall quality at a glance i

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  $\geq 3$ , 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	255	<div> <div>5%</div> <div>59% 30% 9% .</div> </div>
1	C	255	<div> <div>6%</div> <div>60% 32% 5% .</div> </div>
2	B	239	<div> <div>2%</div> <div>64% 28% 8%</div> </div>
2	D	239	<div> <div>3%</div> <div>63% 30% 7%</div> </div>
3	E	251	<div> <div>5%</div> <div>58% 35% 6% .</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	251	
4	F	239	
4	H	239	

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
7	ABU	A	303	-	-	-	X
7	ABU	B	303	-	-	X	X
7	ABU	C	303	-	-	X	-
7	ABU	D	303	-	-	X	X
7	ABU	E	303	-	-	X	X
7	ABU	H	303	-	-	X	X
8	GOL	F	303	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15035 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 Lectin Alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	0	0	0
			1880	1220	294	366			
1	C	249	Total	C	N	O	0	0	0
			1880	1220	294	366			

- Molecule 2 is a protein called Lectin Beta Chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	0	0	0
			1811	1174	284	353			
2	D	239	Total	C	N	O	0	0	0
			1811	1174	284	353			

- Molecule 3 is a protein called Seed lectin alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	249	Total	C	N	O	0	0	0
			1850	1198	289	363			
3	G	249	Total	C	N	O	0	0	0
			1850	1198	289	363			

- Molecule 4 is a protein called Seed lectin beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	239	Total	C	N	O	0	0	0
			1790	1162	277	351			
4	H	239	Total	C	N	O	0	0	0
			1790	1162	277	351			

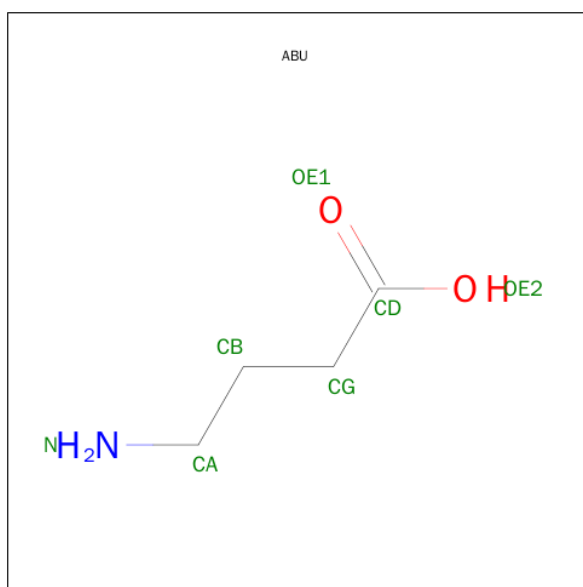
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0
5	E	1	Total Ca 1 1	0	0
5	H	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0
5	A	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Mn 1 1	0	0
6	D	1	Total Mn 1 1	0	0
6	E	1	Total Mn 1 1	0	0
6	H	1	Total Mn 1 1	0	0
6	B	1	Total Mn 1 1	0	0
6	C	1	Total Mn 1 1	0	0
6	A	1	Total Mn 1 1	0	0
6	F	1	Total Mn 1 1	0	0

- Molecule 7 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			7	4	1	2		
7	B	1	Total	C	N	O	0	0
			7	4	1	2		
7	C	1	Total	C	N	O	0	0
			7	4	1	2		
7	D	1	Total	C	N	O	0	0
			7	4	1	2		
7	E	1	Total	C	N	O	0	0
			7	4	1	2		
7	H	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		

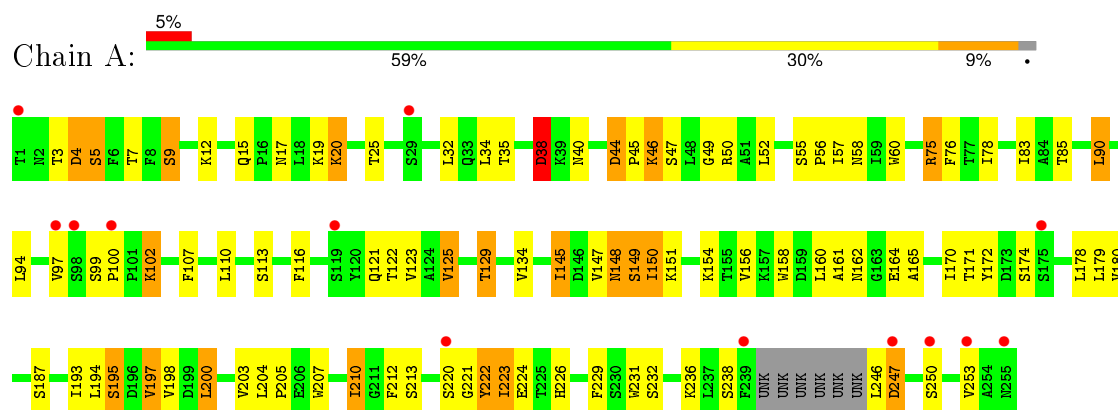
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	33	Total	O	0	0
			33	33		
9	B	39	Total	O	0	0
			39	39		
9	C	36	Total	O	0	0
			36	36		
9	D	34	Total	O	0	0
			34	34		
9	E	40	Total	O	0	0
			40	40		
9	F	35	Total	O	0	0
			35	35		
9	G	42	Total	O	0	0
			42	42		
9	H	38	Total	O	0	0
			38	38		

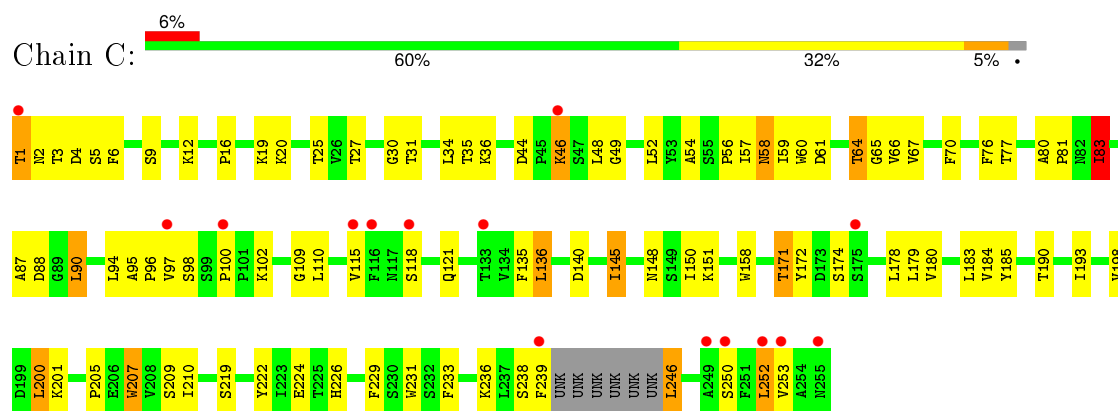
### 3 Residue-property plots

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.

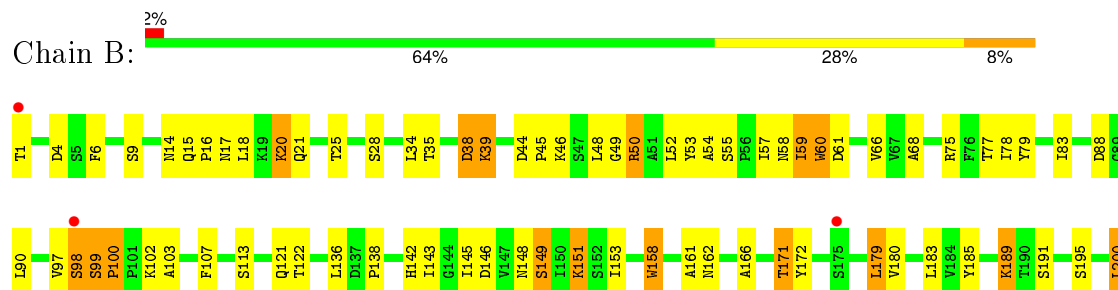
#### • Molecule 1: Lectin Alpha chain



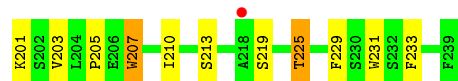
#### • Molecule 1: Lectin Alpha chain



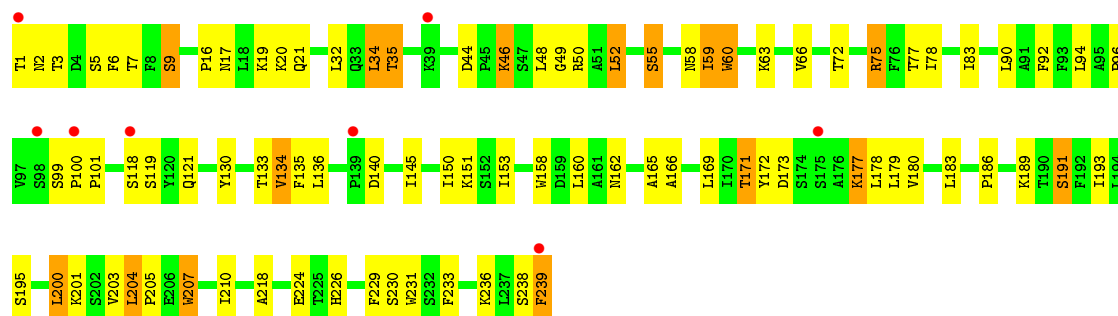
#### • Molecule 2: Lectin Beta Chain



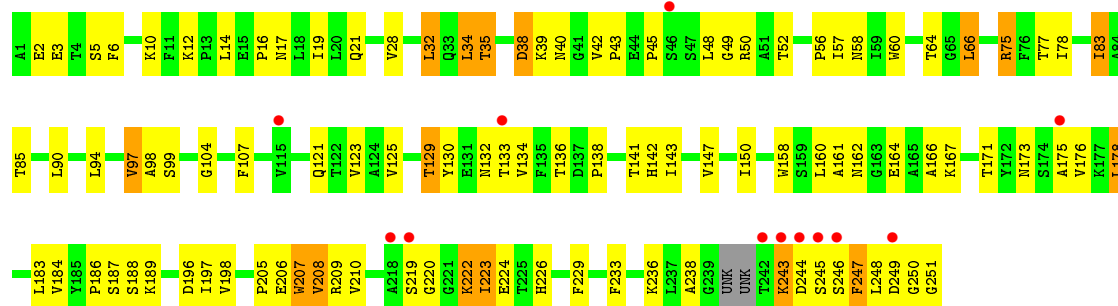




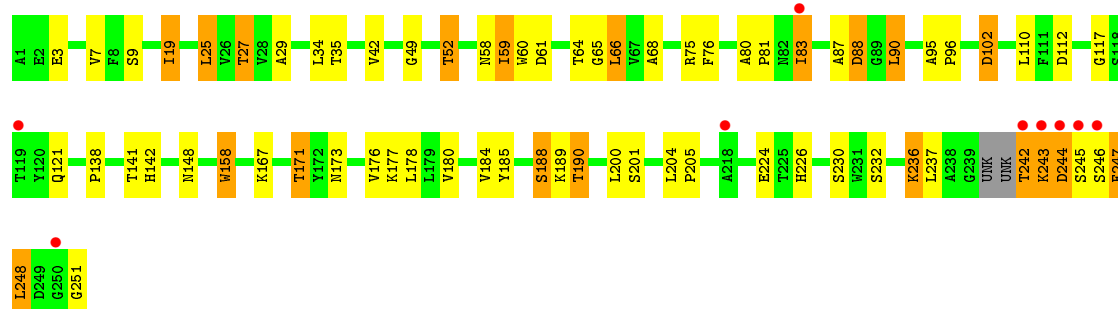
• Molecule 2: Lectin Beta Chain



• Molecule 3: Seed lectin alpha chain

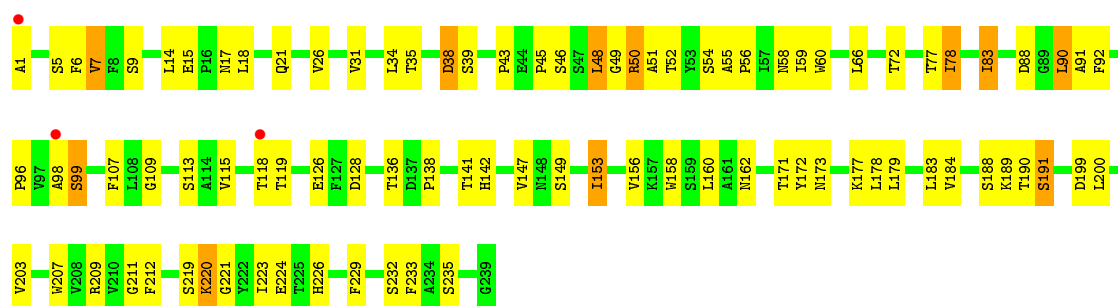


• Molecule 3: Seed lectin alpha chain

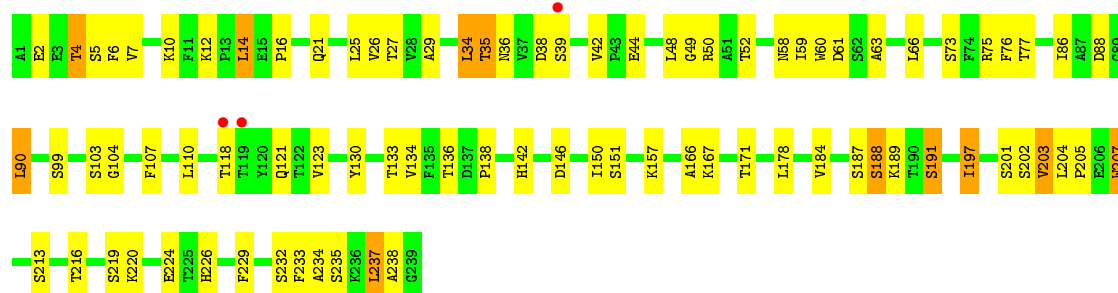


• Molecule 4: Seed lectin beta chain





• Molecule 4: Seed lectin beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.11Å 78.63Å 96.19Å 96.00° 89.99° 100.37°	Depositor
Resolution (Å)	15.84 – 2.50 15.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (15.84-2.50) 92.3 (15.84-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.97 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.211 , 0.289 0.211 , 0.288	Depositor DCC
$R_{free}$ test set	3641 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 72772 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.07 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.3496e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: GOL, CA, MN, ABU

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	0.83	4/1927 (0.2%)	0.93	3/2628 (0.1%)
1	C	0.77	3/1927 (0.2%)	0.84	2/2628 (0.1%)
2	B	0.81	3/1858 (0.2%)	0.94	1/2536 (0.0%)
2	D	0.81	4/1858 (0.2%)	0.90	1/2536 (0.0%)
3	E	0.80	2/1895 (0.1%)	0.88	0/2589
3	G	0.79	2/1895 (0.1%)	0.90	2/2589 (0.1%)
4	F	0.78	1/1836 (0.1%)	0.88	0/2515
4	H	0.82	2/1836 (0.1%)	0.90	2/2515 (0.1%)
All	All	0.80	21/15032 (0.1%)	0.90	11/20536 (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	C	0	1
3	E	0	2
3	G	0	1
4	F	0	1
All	All	0	7

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	ASP	CB-CG	-6.95	1.37	1.51
2	B	60	TRP	CD2-CE2	6.86	1.49	1.41
4	H	60	TRP	CD2-CE2	6.37	1.49	1.41
1	A	60	TRP	CD2-CE2	6.25	1.48	1.41
3	G	158	TRP	CD2-CE2	6.21	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	207	TRP	CD2-CE2	5.96	1.48	1.41
1	A	158	TRP	CD2-CE2	5.93	1.48	1.41
1	A	231	TRP	CD2-CE2	5.66	1.48	1.41
3	E	207	TRP	CD2-CE2	5.54	1.48	1.41
3	E	60	TRP	CD2-CE2	5.46	1.48	1.41
3	G	60	TRP	CD2-CE2	5.43	1.47	1.41
4	H	207	TRP	CD2-CE2	5.37	1.47	1.41
2	D	231	TRP	CD2-CE2	5.29	1.47	1.41
4	F	60	TRP	CD2-CE2	5.29	1.47	1.41
1	C	158	TRP	CD2-CE2	5.28	1.47	1.41
2	D	60	TRP	CD2-CE2	5.18	1.47	1.41
1	C	60	TRP	CD2-CE2	5.18	1.47	1.41
1	C	207	TRP	CD2-CE2	5.16	1.47	1.41
2	B	158	TRP	CD2-CE2	5.13	1.47	1.41
2	D	207	TRP	CD2-CE2	5.12	1.47	1.41
2	D	158	TRP	CD2-CE2	5.06	1.47	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	90	LEU	CA-CB-CG	6.67	130.64	115.30
2	B	66	VAL	CB-CA-C	6.34	123.45	111.40
4	H	237	LEU	CA-CB-CG	6.34	129.88	115.30
1	A	38	ASP	CB-CG-OD2	6.06	123.76	118.30
3	G	25	LEU	CA-CB-CG	6.05	129.22	115.30
3	G	90	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	145	ILE	CG1-CB-CG2	-5.63	99.02	111.40
1	C	136	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	149	SER	CB-CA-C	-5.32	100.00	110.10
2	D	52	LEU	CA-CB-CG	5.28	127.45	115.30
1	C	145	ILE	CB-CA-C	5.05	121.69	111.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ASN	Peptide
1	A	222	TYR	Peptide
1	C	246	LEU	Peptide
3	E	222	LYS	Peptide
3	E	97	VAL	Peptide
4	F	190	THR	Peptide

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Mol	Chain	Res	Type	Group
3	G	246	SER	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	1880	0	1859	89	0
1	C	1880	0	1860	99	0
2	B	1811	0	1794	86	0
2	D	1811	0	1794	77	0
3	E	1850	0	1819	87	0
3	G	1850	0	1819	64	0
4	F	1790	0	1756	65	0
4	H	1790	0	1757	62	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	7	0	5	3	0
7	B	7	0	5	7	0
7	C	7	0	5	10	0
7	D	7	0	5	7	0
7	E	7	0	5	9	0
7	H	7	0	5	8	0
8	C	6	0	8	1	0
8	D	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	6	0	8	1	0
9	A	33	0	0	10	0
9	B	39	0	0	8	0
9	C	36	0	0	12	0
9	D	34	0	0	7	0
9	E	40	0	0	7	0
9	F	35	0	0	4	0
9	G	42	0	0	6	0
9	H	38	0	0	6	0
All	All	15035	0	14512	582	0

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 20.

All (582) 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)
4:H:4:THR:HG22	7:H:303:ABU:HB2	1.23	1.12
1:A:35:THR:HG21	1:A:226:HIS:HD2	1.05	1.11
4:H:4:THR:CG2	7:H:303:ABU:HB2	1.84	1.06
3:G:61:ASP:OD2	3:G:64:THR:HG22	1.53	1.04
1:A:20:LYS:HZ1	1:A:20:LYS:HA	1.21	1.03
2:D:2:ASN:HB3	7:D:303:ABU:HG2	1.41	1.02
1:C:145:ILE:HG21	9:C:436:HOH:O	1.58	1.01
3:E:206:GLU:H	7:E:303:ABU:HG1	1.26	1.00
2:D:239:PHE:HD1	2:D:239:PHE:H	1.03	1.00
1:A:45:PRO:HB2	1:A:46:LYS:HE2	1.46	0.98
2:B:225:THR:HG21	9:B:431:HOH:O	1.61	0.98
1:A:35:THR:HG21	1:A:226:HIS:CD2	1.97	0.97
1:C:64:THR:HG23	1:C:66:VAL:HG23	1.48	0.95
1:C:3:THR:HG22	1:C:236:LYS:HA	1.49	0.94
3:G:188:SER:HB3	3:G:190:THR:HG22	1.49	0.93
3:E:32:LEU:HD13	3:E:34:LEU:HD13	1.50	0.90
1:A:35:THR:CG2	1:A:226:HIS:HD2	1.85	0.90
1:A:35:THR:HG23	9:A:410:HOH:O	1.71	0.89
1:A:20:LYS:NZ	1:A:20:LYS:HA	1.88	0.89
1:A:17:ASN:HD21	7:D:303:ABU:HB1	1.36	0.89
1:C:4:ASP:CB	7:C:303:ABU:OE1	2.20	0.88
3:E:50:ARG:HH22	3:E:99:SER:HB3	1.38	0.88
2:D:145:ILE:HD11	9:D:434:HOH:O	1.73	0.88
1:C:35:THR:OG1	1:C:226:HIS:HD2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:251:GLY:HA2	9:E:438:HOH:O	1.75	0.86
1:C:3:THR:HG21	1:C:236:LYS:HG3	1.55	0.86
1:C:190:THR:HG21	9:C:409:HOH:O	1.75	0.86
2:B:39:LYS:H	2:B:39:LYS:HE2	1.40	0.84
3:G:251:GLY:HA2	9:G:438:HOH:O	1.77	0.84
1:A:247:ASP:HA	9:A:430:HOH:O	1.75	0.84
4:F:191:SER:HB2	9:F:409:HOH:O	1.76	0.84
3:G:173:ASN:HD22	3:G:244:ASP:HA	1.43	0.84
4:F:46:SER:HB2	9:F:435:HOH:O	1.76	0.84
3:G:178:LEU:HD21	4:H:184:VAL:HG11	1.61	0.83
4:F:220:LYS:HE2	4:F:221:GLY:H	1.42	0.82
1:C:3:THR:CG2	1:C:236:LYS:HG3	2.09	0.82
1:C:4:ASP:HB2	7:C:303:ABU:OE1	1.80	0.81
1:C:27:THR:HG22	1:C:31:THR:H	1.41	0.81
3:E:176:VAL:HG23	3:E:178:LEU:HB2	1.62	0.80
3:E:251:GLY:C	9:E:438:HOH:O	2.18	0.80
3:E:196:ASP:OD1	4:F:189:LYS:HE2	1.80	0.80
1:C:145:ILE:HD13	9:C:436:HOH:O	1.81	0.80
3:E:206:GLU:N	7:E:303:ABU:HG1	1.96	0.79
2:B:171:THR:HG22	9:B:416:HOH:O	1.82	0.79
3:G:59:ILE:HD13	3:G:68:ALA:HB3	1.65	0.78
1:A:236:LYS:HZ2	1:A:246:LEU:N	1.81	0.78
2:D:239:PHE:HD1	2:D:239:PHE:N	1.82	0.78
3:E:251:GLY:CA	9:E:438:HOH:O	2.30	0.78
2:B:97:VAL:O	2:B:98:SER:HB2	1.83	0.78
2:B:136:LEU:HD13	2:B:151:LYS:HE2	1.66	0.78
3:G:243:LYS:HG2	3:G:244:ASP:H	1.49	0.78
1:A:9:SER:HB2	2:D:1:THR:N	1.99	0.78
3:G:7:VAL:HG22	3:G:232:SER:HB2	1.66	0.77
1:A:57:ILE:HG13	1:A:210:ILE:CD1	2.13	0.77
2:B:79:TYR:H	2:B:225:THR:HG22	1.50	0.77
1:A:20:LYS:NZ	1:A:20:LYS:CA	2.48	0.76
2:D:59:ILE:HD11	2:D:205:PRO:O	1.85	0.76
1:A:107:PHE:HE1	1:A:113:SER:HA	1.51	0.76
3:E:97:VAL:HG13	3:E:209:ARG:NH1	2.01	0.75
2:B:16:PRO:HB2	1:C:56:PRO:HG2	1.66	0.75
2:B:145:ILE:HD11	9:B:439:HOH:O	1.87	0.74
3:G:173:ASN:HB2	3:G:244:ASP:HB3	1.68	0.74
2:B:15:GLN:HE21	2:B:18:LEU:HG	1.51	0.74
3:E:219:SER:HA	9:E:405:HOH:O	1.88	0.74
1:A:145:ILE:CD1	9:A:433:HOH:O	2.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:SER:HG	8:C:304:GOL:HO1	1.25	0.74
2:B:98:SER:HB2	9:B:428:HOH:O	1.86	0.74
2:D:171:THR:HG22	9:D:412:HOH:O	1.87	0.74
4:F:220:LYS:HE2	4:F:221:GLY:N	2.02	0.73
1:C:145:ILE:HD12	1:C:179:LEU:HD23	1.71	0.73
1:A:180:VAL:HG22	1:A:195:SER:HB3	1.69	0.73
3:G:184:VAL:HG11	4:H:178:LEU:HD21	1.71	0.73
2:B:15:GLN:NE2	2:B:18:LEU:HG	2.04	0.73
2:B:58:ASN:H	7:B:303:ABU:HB2	1.54	0.73
7:A:303:ABU:CA	2:D:17:ASN:HD21	2.02	0.73
1:C:184:VAL:HG11	2:D:178:LEU:HD21	1.71	0.72
4:F:98:ALA:H	4:F:209:ARG:HH11	1.37	0.72
1:C:172:TYR:CE2	1:C:200:LEU:HD22	2.25	0.72
1:A:58:ASN:N	7:A:303:ABU:OE1	2.21	0.71
2:B:21:GLN:OE1	2:B:50:ARG:HD3	1.90	0.71
1:C:27:THR:CG2	1:C:31:THR:H	2.02	0.71
1:C:83:ILE:HD12	1:C:83:ILE:H	1.54	0.71
1:A:57:ILE:HG13	1:A:210:ILE:HD13	1.70	0.71
4:F:52:THR:HG21	4:F:209:ARG:HD3	1.72	0.71
1:C:58:ASN:HB2	7:C:303:ABU:HE2	1.73	0.70
1:A:55:SER:OG	2:D:55:SER:HB3	1.91	0.70
4:F:83:ILE:HG12	4:F:162:ASN:ND2	2.05	0.70
1:C:4:ASP:HB3	7:C:303:ABU:OE1	1.91	0.70
2:B:46:LYS:NZ	2:B:46:LYS:HB2	2.05	0.70
2:D:83:ILE:HD11	2:D:160:LEU:HD23	1.74	0.70
2:D:78:ILE:HG23	2:D:224:GLU:HG3	1.73	0.70
2:B:4:ASP:HB2	7:B:303:ABU:HB1	1.74	0.69
3:G:173:ASN:ND2	3:G:244:ASP:HA	2.07	0.69
2:D:145:ILE:CG1	9:D:434:HOH:O	2.40	0.69
2:B:136:LEU:CD1	2:B:151:LYS:HE2	2.23	0.67
1:A:145:ILE:HD11	9:A:433:HOH:O	1.94	0.67
1:A:107:PHE:CE1	1:A:113:SER:HA	2.30	0.67
2:B:34:LEU:O	2:B:49:GLY:HA3	1.95	0.67
2:B:57:ILE:HG22	7:B:303:ABU:OE1	1.95	0.67
1:C:27:THR:HG22	1:C:31:THR:N	2.10	0.67
3:E:43:PRO:HG2	3:E:223:ILE:HG23	1.76	0.67
1:C:4:ASP:OD2	1:C:57:ILE:HD12	1.95	0.66
3:G:251:GLY:CA	9:G:438:HOH:O	2.37	0.66
3:G:178:LEU:HD21	4:H:184:VAL:CG1	2.25	0.66
3:E:129:THR:HG21	3:E:224:GLU:OE2	1.95	0.66
1:A:57:ILE:CG1	1:A:210:ILE:HD13	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:LYS:HB3	1:C:236:LYS:NZ	2.11	0.65
2:D:48:LEU:HD23	2:D:49:GLY:N	2.12	0.65
3:E:75:ARG:HA	3:E:166:ALA:O	1.97	0.65
9:B:403:HOH:O	7:C:303:ABU:HB2	1.96	0.65
2:B:97:VAL:O	2:B:98:SER:CB	2.45	0.65
3:E:205:PRO:CB	7:E:303:ABU:HG2	2.26	0.65
3:E:77:THR:HG1	3:E:229:PHE:HZ	1.39	0.64
4:F:45:PRO:HG3	4:F:220:LYS:HE3	1.80	0.64
3:G:35:THR:OG1	3:G:226:HIS:HD2	1.80	0.64
3:G:242:THR:N	4:H:232:SER:HG	1.96	0.64
3:E:58:ASN:HD21	4:H:12:LYS:NZ	1.95	0.64
1:A:9:SER:HB2	2:D:1:THR:H3	1.60	0.64
4:F:35:THR:OG1	4:F:226:HIS:HD2	1.81	0.64
1:A:200:LEU:HG	1:A:204:LEU:HD12	1.79	0.64
1:A:78:ILE:HG23	1:A:224:GLU:HG3	1.80	0.63
1:A:35:THR:OG1	1:A:47:SER:HB3	1.97	0.63
2:D:46:LYS:HE2	2:D:218:ALA:HA	1.80	0.63
2:B:77:THR:HB	2:B:229:PHE:HZ	1.63	0.63
1:A:145:ILE:HG13	9:A:433:HOH:O	1.98	0.63
1:A:5:SER:HB3	2:D:5:SER:HB3	1.81	0.63
3:E:17:ASN:ND2	7:H:303:ABU:OE1	2.20	0.63
4:F:98:ALA:H	4:F:209:ARG:NH1	1.97	0.63
4:H:34:LEU:O	4:H:49:GLY:HA3	1.99	0.63
2:B:205:PRO:HG2	2:B:207:TRP:O	1.99	0.62
1:C:171:THR:HG21	8:D:304:GOL:H2	1.80	0.62
1:A:50:ARG:HA	1:A:212:PHE:O	1.99	0.62
1:C:46:LYS:NZ	1:C:46:LYS:HB3	2.14	0.62
3:G:188:SER:HB3	3:G:190:THR:CG2	2.27	0.62
3:G:27:THR:CG2	3:G:29:ALA:H	2.12	0.62
2:D:172:TYR:CE2	2:D:200:LEU:HD22	2.35	0.62
2:B:83:ILE:HD13	2:B:162:ASN:HB2	1.80	0.62
1:A:45:PRO:N	1:A:223:ILE:HD11	2.14	0.62
3:E:121:GLN:HB3	3:E:205:PRO:HD3	1.81	0.62
3:E:129:THR:HG21	3:E:224:GLU:CD	2.20	0.62
4:H:58:ASN:H	7:H:303:ABU:HB1	1.65	0.62
2:B:77:THR:HB	2:B:229:PHE:CZ	2.34	0.62
3:E:176:VAL:CG2	3:E:178:LEU:HB2	2.29	0.61
4:H:5:SER:HB3	4:H:234:ALA:HA	1.82	0.61
3:E:32:LEU:HD13	3:E:34:LEU:CD1	2.28	0.61
1:C:64:THR:CG2	1:C:66:VAL:H	2.14	0.61
1:A:154:LYS:HG2	1:A:194:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:THR:HG21	9:C:424:HOH:O	2.00	0.61
1:A:9:SER:CB	2:D:1:THR:N	2.63	0.61
3:E:57:ILE:HD13	3:E:233:PHE:CE2	2.36	0.61
2:B:79:TYR:H	2:B:225:THR:CG2	2.13	0.61
3:E:50:ARG:HH22	3:E:99:SER:CB	2.10	0.61
1:C:61:ASP:OD2	1:C:64:THR:HB	2.01	0.61
3:E:141:THR:HG22	3:E:158:TRP:O	2.01	0.61
2:B:39:LYS:N	2:B:39:LYS:HE2	2.13	0.60
2:B:50:ARG:HG2	2:B:213:SER:HB2	1.81	0.60
1:C:178:LEU:HD22	2:D:186:PRO:HA	1.83	0.60
3:G:245:SER:O	3:G:248:LEU:HB2	2.01	0.60
3:E:98:ALA:HB2	3:E:209:ARG:NH1	2.16	0.60
3:G:243:LYS:HE3	3:G:244:ASP:OD2	2.01	0.60
2:B:171:THR:CG2	9:B:416:HOH:O	2.46	0.59
3:E:32:LEU:CD1	3:E:34:LEU:HD13	2.28	0.59
1:C:34:LEU:O	1:C:49:GLY:HA3	2.01	0.59
4:H:235:SER:HG	7:H:303:ABU:N	2.00	0.59
3:E:207:TRP:H	7:E:303:ABU:HB2	1.68	0.59
1:C:46:LYS:HG2	1:C:46:LYS:O	2.01	0.59
3:G:243:LYS:HB2	4:H:73:SER:OG	2.03	0.59
4:F:149:SER:HA	9:F:412:HOH:O	2.01	0.59
3:E:129:THR:HG21	3:E:224:GLU:OE1	2.03	0.58
2:D:96:PRO:O	2:D:99:SER:HB3	2.02	0.58
3:G:87:ALA:HB1	3:G:88:ASP:OD1	2.03	0.58
1:C:95:ALA:HB1	1:C:96:PRO:HD2	1.85	0.58
4:F:138:PRO:HD2	4:F:142:HIS:CE1	2.38	0.58
3:E:21:GLN:NE2	3:E:50:ARG:HE	2.00	0.58
3:E:58:ASN:HD21	4:H:12:LYS:HZ3	1.52	0.58
4:H:50:ARG:HG2	4:H:213:SER:HB2	1.86	0.58
1:A:221:GLY:HA3	9:A:414:HOH:O	2.03	0.58
4:F:17:ASN:O	4:F:54:SER:HB2	2.03	0.58
3:E:224:GLU:OE2	3:E:226:HIS:HE1	1.86	0.57
3:G:27:THR:HG23	3:G:29:ALA:H	1.69	0.57
2:D:121:GLN:HB3	2:D:205:PRO:HD3	1.86	0.57
1:C:61:ASP:O	1:C:65:GLY:N	2.36	0.57
3:G:178:LEU:CD2	4:H:184:VAL:HG11	2.34	0.57
1:A:17:ASN:ND2	7:D:303:ABU:OE2	2.38	0.57
2:B:146:ASP:HB3	2:B:149:SER:O	2.05	0.57
1:A:156:VAL:HG22	9:A:409:HOH:O	2.04	0.57
4:H:4:THR:HG22	7:H:303:ABU:CB	2.16	0.56
3:E:224:GLU:OE2	3:E:226:HIS:CE1	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ASN:CB	7:C:303:ABU:HE2	2.36	0.56
4:H:88:ASP:HB3	9:H:406:HOH:O	2.05	0.56
3:G:83:ILE:H	3:G:83:ILE:HD12	1.70	0.56
3:E:56:PRO:HB3	3:E:97:VAL:HG21	1.88	0.56
1:A:7:THR:HB	2:D:3:THR:HB	1.88	0.56
3:G:138:PRO:HD2	3:G:142:HIS:CE1	2.41	0.56
3:E:32:LEU:CD1	3:E:34:LEU:CD1	2.84	0.56
1:A:9:SER:HB2	2:D:1:THR:H2	1.69	0.56
1:A:197:VAL:CG1	2:B:189:LYS:HD2	2.35	0.56
3:G:200:LEU:HG	3:G:204:LEU:HD12	1.87	0.56
1:A:56:PRO:HG2	2:D:16:PRO:HB2	1.88	0.56
2:B:122:THR:H	2:B:148:ASN:ND2	2.04	0.55
3:E:3:GLU:O	4:H:6:PHE:HA	2.07	0.55
1:C:27:THR:HG23	1:C:30:GLY:H	1.72	0.55
1:C:46:LYS:CG	1:C:46:LYS:O	2.55	0.55
4:F:50:ARG:HB3	4:F:212:PHE:O	2.05	0.55
1:C:2:ASN:HB3	7:C:303:ABU:HB1	1.88	0.55
1:C:219:SER:O	1:C:222:TYR:HB2	2.05	0.55
3:E:50:ARG:NH2	3:E:99:SER:HB3	2.18	0.55
2:B:138:PRO:HD2	2:B:142:HIS:CE1	2.42	0.55
3:G:19:ILE:HG13	3:G:52:THR:HG22	1.88	0.55
3:E:130:TYR:HD2	3:E:132:ASN:ND2	2.05	0.55
2:B:100:PRO:HD2	2:B:102:LYS:NZ	2.22	0.55
3:G:176:VAL:O	3:G:177:LYS:HB2	2.07	0.54
2:D:59:ILE:CD1	2:D:205:PRO:O	2.55	0.54
4:H:27:THR:OG1	4:H:29:ALA:HB3	2.07	0.54
4:H:191:SER:HB2	9:H:409:HOH:O	2.06	0.54
1:A:172:TYR:CE2	1:A:200:LEU:HD22	2.43	0.54
3:G:245:SER:O	3:G:248:LEU:HG	2.08	0.54
2:D:50:ARG:HD2	2:D:101:PRO:HG3	1.88	0.54
1:C:48:LEU:HD11	1:C:109:GLY:HA3	1.90	0.54
1:A:164:GLU:HG2	1:A:187:SER:OG	2.07	0.54
3:G:27:THR:HG22	3:G:29:ALA:N	2.22	0.54
2:D:173:ASP:O	2:D:177:LYS:N	2.40	0.54
2:D:2:ASN:HB3	7:D:303:ABU:CG	2.27	0.54
2:D:46:LYS:CE	2:D:218:ALA:HA	2.37	0.54
1:C:121:GLN:HB3	1:C:205:PRO:HD3	1.88	0.54
2:B:14:ASN:O	2:B:15:GLN:HB3	2.07	0.54
1:A:145:ILE:CG1	9:A:433:HOH:O	2.54	0.54
2:B:55:SER:OG	1:C:54:ALA:HB3	2.08	0.54
1:C:64:THR:HG23	1:C:66:VAL:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:19:ILE:HB	3:E:52:THR:CG2	2.38	0.54
4:F:156:VAL:HG22	9:F:425:HOH:O	2.08	0.54
4:F:77:THR:HG1	4:F:229:PHE:HZ	1.52	0.53
2:B:121:GLN:HA	2:B:203:VAL:O	2.08	0.53
3:E:205:PRO:HB2	7:E:303:ABU:HG2	1.89	0.53
3:G:42:VAL:HG22	9:G:425:HOH:O	2.08	0.53
1:C:236:LYS:HZ3	1:C:236:LYS:HB3	1.72	0.53
2:D:172:TYR:CZ	2:D:200:LEU:HD22	2.44	0.53
4:H:21:GLN:OE1	4:H:50:ARG:HD3	2.08	0.53
4:F:17:ASN:HA	4:F:54:SER:HB2	1.90	0.53
2:B:172:TYR:CE2	2:B:200:LEU:HD22	2.43	0.53
2:B:58:ASN:HB2	7:B:303:ABU:CA	2.39	0.53
1:C:83:ILE:H	1:C:83:ILE:CD1	2.16	0.53
1:A:193:ILE:HG23	2:B:191:SER:OG	2.08	0.53
1:C:135:PHE:O	1:C:151:LYS:HG2	2.09	0.53
3:E:245:SER:C	3:E:247:PHE:H	2.12	0.53
3:G:76:PHE:CD1	3:G:90:LEU:HD21	2.44	0.53
1:A:149:SER:OG	1:A:150:ILE:N	2.39	0.53
1:A:15:GLN:HE22	7:D:303:ABU:CA	2.21	0.53
1:C:83:ILE:N	1:C:83:ILE:HD12	2.21	0.53
4:F:78:ILE:HD12	4:F:224:GLU:CG	2.38	0.53
1:C:121:GLN:N	1:C:148:ASN:HD21	2.07	0.53
2:B:78:ILE:HA	2:B:225:THR:HG22	1.90	0.53
1:C:6:PHE:CZ	1:C:233:PHE:HB3	2.44	0.53
4:H:136:THR:O	4:H:136:THR:HG22	2.08	0.52
4:F:199:ASP:O	4:F:203:VAL:HG22	2.09	0.52
2:D:75:ARG:HA	2:D:166:ALA:O	2.10	0.52
4:H:59:ILE:HD11	4:H:205:PRO:O	2.09	0.52
4:H:77:THR:HB	4:H:229:PHE:CZ	2.44	0.52
3:E:164:GLU:HG3	3:E:187:SER:OG	2.09	0.52
2:D:239:PHE:N	2:D:239:PHE:CD1	2.54	0.52
2:B:57:ILE:CG2	7:B:303:ABU:OE1	2.58	0.52
4:H:121:GLN:HB3	4:H:205:PRO:HD3	1.90	0.52
1:A:34:LEU:O	1:A:49:GLY:HA3	2.08	0.52
1:A:129:THR:HG21	1:A:224:GLU:OE2	2.09	0.52
8:D:304:GOL:H31	9:D:430:HOH:O	2.09	0.52
4:F:58:ASN:HB2	4:F:207:TRP:CH2	2.44	0.52
4:F:7:VAL:HB	4:F:232:SER:HB3	1.92	0.52
3:E:205:PRO:HB3	7:E:303:ABU:HG2	1.92	0.52
1:A:122:THR:H	1:A:148:ASN:ND2	2.07	0.52
2:B:17:ASN:HA	2:B:54:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:184:VAL:HG11	4:H:178:LEU:CD2	2.40	0.51
2:D:145:ILE:CD1	9:D:434:HOH:O	2.39	0.51
2:B:145:ILE:HD12	2:B:179:LEU:CD1	2.41	0.51
4:F:224:GLU:OE2	4:F:226:HIS:HE1	1.94	0.51
2:D:48:LEU:C	2:D:48:LEU:HD23	2.30	0.51
3:G:102:ASP:HB2	3:G:112:ASP:OD1	2.10	0.51
2:B:17:ASN:ND2	7:C:303:ABU:HG2	2.25	0.51
2:B:207:TRP:CZ2	1:C:16:PRO:HD2	2.45	0.51
1:C:96:PRO:HB3	9:C:411:HOH:O	2.11	0.51
4:H:75:ARG:HA	4:H:166:ALA:O	2.10	0.51
8:F:303:GOL:O1	8:F:303:GOL:O3	2.23	0.51
2:B:79:TYR:N	2:B:225:THR:HG22	2.22	0.51
1:A:102:LYS:HG3	1:A:110:LEU:C	2.31	0.51
4:H:104:GLY:O	4:H:107:PHE:HD2	1.93	0.51
3:E:34:LEU:O	3:E:49:GLY:HA3	2.11	0.51
1:A:20:LYS:HZ2	1:A:20:LYS:CA	2.24	0.51
3:G:34:LEU:O	3:G:49:GLY:HA3	2.11	0.51
1:A:17:ASN:ND2	7:D:303:ABU:HB1	2.17	0.51
1:A:38:ASP:OD2	1:A:38:ASP:C	2.48	0.51
2:B:103:ALA:O	2:B:107:PHE:HB2	2.11	0.51
3:E:12:LYS:NZ	4:H:61:ASP:OD1	2.41	0.51
1:C:193:ILE:HG23	2:D:191:SER:HB3	1.92	0.51
1:A:35:THR:CG2	1:A:226:HIS:CD2	2.76	0.50
1:C:236:LYS:HB2	1:C:246:LEU:HD13	1.92	0.50
2:D:66:VAL:HG21	2:D:238:SER:O	2.11	0.50
2:D:2:ASN:CB	7:D:303:ABU:HG2	2.29	0.50
3:G:243:LYS:CG	3:G:244:ASP:H	2.18	0.50
4:F:78:ILE:HG12	4:F:160:LEU:HD11	1.92	0.50
2:B:145:ILE:HD12	2:B:179:LEU:HD13	1.93	0.50
4:F:17:ASN:C	4:F:54:SER:HB2	2.31	0.50
1:A:205:PRO:HG2	1:A:207:TRP:O	2.11	0.50
1:C:150:ILE:HG13	9:C:407:HOH:O	2.10	0.50
3:E:78:ILE:HD11	3:E:160:LEU:HD13	1.93	0.50
2:D:136:LEU:HD22	2:D:151:LYS:HD3	1.94	0.50
3:E:183:LEU:HD23	3:E:183:LEU:C	2.32	0.50
1:A:107:PHE:HE1	1:A:113:SER:CA	2.23	0.50
4:H:7:VAL:HG22	4:H:232:SER:HB2	1.94	0.50
2:B:60:TRP:CE3	2:B:201:LYS:HG3	2.46	0.50
2:B:46:LYS:HZ3	2:B:46:LYS:HB2	1.77	0.50
2:D:77:THR:HG1	2:D:229:PHE:HE1	1.51	0.50
4:F:141:THR:OG1	4:F:158:TRP:O	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:THR:HG21	9:C:435:HOH:O	2.11	0.50
1:A:57:ILE:CG1	1:A:210:ILE:CD1	2.85	0.50
4:H:2:GLU:HB3	7:H:303:ABU:CG	2.41	0.49
1:C:5:SER:HB2	1:C:233:PHE:O	2.12	0.49
1:A:102:LYS:HZ2	1:A:102:LYS:HA	1.76	0.49
3:E:184:VAL:HG11	4:F:178:LEU:HD21	1.93	0.49
1:A:224:GLU:OE2	1:A:226:HIS:CE1	2.65	0.49
1:A:9:SER:CB	2:D:1:THR:H3	2.22	0.49
2:B:58:ASN:H	7:B:303:ABU:CB	2.21	0.49
1:A:149:SER:C	1:A:151:LYS:H	2.15	0.49
4:H:224:GLU:OE2	4:H:226:HIS:HE1	1.94	0.49
3:E:206:GLU:H	7:E:303:ABU:CD	2.25	0.49
2:B:17:ASN:HD21	7:C:303:ABU:HG2	1.77	0.49
3:E:243:LYS:HB2	3:G:236:LYS:HD2	1.94	0.49
1:A:20:LYS:CB	1:A:20:LYS:NZ	2.74	0.49
2:D:150:ILE:HG13	9:D:425:HOH:O	2.12	0.49
3:E:186:PRO:HD2	9:E:414:HOH:O	2.11	0.49
1:C:2:ASN:HD22	7:C:303:ABU:N	2.11	0.49
2:B:45:PRO:HB2	2:B:46:LYS:HE3	1.95	0.49
4:H:5:SER:HB2	4:H:233:PHE:O	2.13	0.49
3:G:83:ILE:H	3:G:83:ILE:CD1	2.23	0.49
2:B:46:LYS:HZ2	2:B:46:LYS:HB2	1.76	0.49
1:A:224:GLU:OE2	1:A:226:HIS:HE1	1.96	0.49
1:C:224:GLU:OE2	1:C:226:HIS:HE1	1.95	0.49
3:G:27:THR:CG2	3:G:29:ALA:N	2.74	0.49
1:C:193:ILE:HG22	2:D:193:ILE:HG22	1.95	0.49
3:G:173:ASN:HD22	3:G:244:ASP:CA	2.21	0.49
1:C:252:LEU:HD12	2:D:169:LEU:HD21	1.93	0.49
1:C:83:ILE:HG23	9:C:408:HOH:O	2.12	0.48
3:E:2:GLU:HG2	9:E:420:HOH:O	2.13	0.48
3:E:248:LEU:C	3:E:250:GLY:H	2.15	0.48
2:B:58:ASN:HB3	7:B:303:ABU:HG2	1.96	0.48
1:C:172:TYR:CZ	1:C:200:LEU:HD22	2.48	0.48
3:E:6:PHE:CZ	3:E:233:PHE:HB3	2.48	0.48
3:E:164:GLU:CG	3:E:187:SER:OG	2.61	0.48
1:A:164:GLU:CG	1:A:187:SER:OG	2.62	0.48
1:C:210:ILE:HD13	1:C:231:TRP:HZ2	1.79	0.48
4:H:86:ILE:O	4:H:130:TYR:HB2	2.13	0.48
3:E:196:ASP:OD1	4:F:189:LYS:CE	2.58	0.48
1:C:46:LYS:HZ3	1:C:46:LYS:HB3	1.78	0.48
1:C:1:THR:HG22	1:C:239:PHE:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:121:GLN:N	3:G:148:ASN:ND2	2.62	0.48
3:E:38:ASP:OD1	3:E:42:VAL:HB	2.13	0.48
3:E:38:ASP:OD2	3:E:40:ASN:HB2	2.13	0.48
1:C:145:ILE:CG2	9:C:436:HOH:O	2.35	0.48
3:E:19:ILE:HB	3:E:52:THR:HG22	1.95	0.48
4:H:201:SER:HB2	9:H:421:HOH:O	2.14	0.48
1:C:236:LYS:CB	1:C:236:LYS:NZ	2.73	0.48
4:F:147:VAL:HG21	4:F:153:ILE:HD11	1.96	0.48
2:D:183:LEU:HD23	2:D:183:LEU:C	2.34	0.48
1:A:19:LYS:HB2	1:A:52:LEU:CD1	2.44	0.48
2:B:79:TYR:HB3	2:B:225:THR:HB	1.95	0.47
1:C:94:LEU:HG	1:C:210:ILE:HG22	1.96	0.47
2:D:134:VAL:HG22	2:D:135:PHE:CD1	2.48	0.47
1:C:77:THR:HG1	1:C:229:PHE:HZ	1.57	0.47
2:D:6:PHE:HZ	2:D:210:ILE:HD11	1.78	0.47
4:H:77:THR:OG1	4:H:229:PHE:CE1	2.68	0.47
2:B:9:SER:CB	1:C:1:THR:H2	2.27	0.47
1:A:55:SER:OG	2:D:55:SER:CB	2.60	0.47
4:F:17:ASN:CA	4:F:54:SER:HB2	2.44	0.47
4:F:43:PRO:HG2	4:F:223:ILE:HD12	1.96	0.47
1:A:3:THR:HB	2:D:7:THR:HB	1.95	0.47
4:H:42:VAL:HG21	9:H:420:HOH:O	2.14	0.47
2:D:59:ILE:HD13	2:D:60:TRP:HD1	1.80	0.47
2:B:15:GLN:HE21	2:B:18:LEU:CG	2.23	0.47
2:B:100:PRO:HD2	2:B:102:LYS:HZ1	1.78	0.47
4:F:77:THR:HB	4:F:229:PHE:HZ	1.79	0.47
2:D:77:THR:OG1	2:D:229:PHE:CZ	2.66	0.47
1:C:35:THR:OG1	1:C:226:HIS:CD2	2.50	0.47
3:G:243:LYS:HG2	3:G:244:ASP:N	2.24	0.47
3:G:121:GLN:HB3	3:G:205:PRO:HD3	1.96	0.47
2:B:39:LYS:CE	2:B:39:LYS:H	2.20	0.47
3:E:138:PRO:HD2	3:E:142:HIS:CE1	2.49	0.47
3:E:66:LEU:HD22	3:E:238:ALA:O	2.15	0.47
4:F:78:ILE:HD12	4:F:224:GLU:CD	2.35	0.47
4:F:38:ASP:OD1	4:F:38:ASP:C	2.53	0.47
4:H:123:VAL:HA	4:H:146:ASP:O	2.15	0.47
3:G:224:GLU:HG3	3:G:226:HIS:CE1	2.50	0.46
3:E:236:LYS:HE2	3:E:245:SER:O	2.14	0.46
3:G:141:THR:OG1	3:G:158:TRP:O	2.27	0.46
2:D:34:LEU:O	2:D:49:GLY:HA3	2.15	0.46
3:E:78:ILE:CD1	3:E:158:TRP:HH2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:THR:HB	1:C:238:SER:HA	1.96	0.46
3:E:104:GLY:O	3:E:107:PHE:HD2	1.98	0.46
4:H:36:ASN:HB2	4:H:44:GLU:HB2	1.97	0.46
1:C:185:TYR:HD2	1:C:190:THR:HG23	1.81	0.46
2:B:145:ILE:CD1	9:B:439:HOH:O	2.55	0.46
4:F:78:ILE:HD12	4:F:224:GLU:HG3	1.97	0.46
2:B:83:ILE:HD13	2:B:162:ASN:CB	2.45	0.46
1:C:96:PRO:CG	9:C:411:HOH:O	2.63	0.46
2:B:1:THR:N	1:C:9:SER:HB2	2.29	0.46
3:E:143:ILE:HG13	3:E:158:TRP:HB2	1.97	0.46
4:H:203:VAL:CG1	4:H:203:VAL:O	2.64	0.46
4:F:90:LEU:HD12	4:F:90:LEU:C	2.36	0.46
2:B:98:SER:O	2:B:99:SER:C	2.54	0.46
3:E:75:ARG:HG3	3:E:229:PHE:HD2	1.81	0.46
2:B:83:ILE:CD1	2:B:162:ASN:HB2	2.46	0.46
1:C:252:LEU:HA	1:C:252:LEU:HD23	1.83	0.46
2:D:145:ILE:HD13	2:D:179:LEU:HD23	1.97	0.46
3:E:183:LEU:HD23	3:E:184:VAL:N	2.30	0.46
3:G:117:GLY:HA3	9:G:424:HOH:O	2.15	0.46
2:D:180:VAL:HG22	2:D:195:SER:HB2	1.98	0.46
4:F:220:LYS:HE2	4:F:220:LYS:CA	2.45	0.46
4:H:121:GLN:HG2	9:H:437:HOH:O	2.16	0.45
1:C:210:ILE:HD13	1:C:231:TRP:CZ2	2.52	0.45
1:C:250:SER:HA	1:C:253:VAL:HG12	1.97	0.45
2:B:20:LYS:HB3	2:B:20:LYS:HE3	1.61	0.45
4:F:7:VAL:HG13	3:G:3:GLU:HB2	1.98	0.45
3:G:121:GLN:CA	3:G:148:ASN:HD21	2.30	0.45
1:A:83:ILE:HD13	1:A:162:ASN:HB2	1.99	0.45
2:B:75:ARG:HA	2:B:166:ALA:O	2.16	0.45
2:B:38:ASP:OD1	2:B:38:ASP:C	2.55	0.45
3:E:75:ARG:HE	3:E:167:LYS:NZ	2.15	0.45
4:H:58:ASN:ND2	4:H:207:TRP:CZ2	2.85	0.45
1:C:64:THR:CG2	1:C:66:VAL:HG23	2.33	0.45
1:C:70:PHE:HA	1:C:246:LEU:HD21	1.99	0.45
2:B:210:ILE:HD12	2:B:231:TRP:HZ2	1.80	0.45
4:H:14:LEU:HD22	4:H:16:PRO:HG3	1.99	0.45
2:D:20:LYS:HB2	2:D:20:LYS:NZ	2.32	0.45
1:C:27:THR:HG23	1:C:30:GLY:N	2.30	0.45
4:F:173:ASN:O	4:F:177:LYS:N	2.48	0.45
3:G:189:LYS:HD3	4:H:197:ILE:HD11	1.99	0.45
1:C:1:THR:HG22	1:C:239:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:126:GLU:OE2	4:F:128:ASP:HB2	2.16	0.45
4:H:76:PHE:CG	4:H:90:LEU:HD21	2.52	0.45
4:H:35:THR:HG21	4:H:216:THR:CG2	2.47	0.45
3:E:21:GLN:HE22	3:E:50:ARG:HH21	1.64	0.45
2:B:210:ILE:HD13	2:B:233:PHE:CD1	2.51	0.45
3:G:171:THR:HG22	3:G:180:VAL:HB	1.98	0.45
1:A:76:PHE:CE1	1:A:90:LEU:HD21	2.52	0.44
1:C:96:PRO:HD3	9:C:411:HOH:O	2.17	0.44
4:H:77:THR:OG1	4:H:229:PHE:HE1	1.99	0.44
1:C:76:PHE:CD1	1:C:90:LEU:HD21	2.53	0.44
3:G:244:ASP:OD2	4:H:167:LYS:HD3	2.17	0.44
4:H:187:SER:O	4:H:188:SER:CB	2.66	0.44
1:A:45:PRO:HG3	1:A:220:SER:HB3	2.00	0.44
4:F:77:THR:HB	4:F:229:PHE:CZ	2.53	0.44
1:A:12:LYS:NZ	2:D:58:ASN:HD21	2.15	0.44
2:D:58:ASN:HB2	2:D:207:TRP:CH2	2.52	0.44
2:D:72:THR:HG21	2:D:92:PHE:CZ	2.53	0.44
1:C:67:VAL:HB	1:C:174:SER:HB2	1.98	0.44
4:H:2:GLU:HB3	7:H:303:ABU:OE2	2.18	0.44
2:B:17:ASN:O	2:B:54:ALA:N	2.50	0.44
3:G:242:THR:HG23	3:G:247:PHE:HA	1.99	0.44
4:H:50:ARG:HG2	4:H:213:SER:CB	2.48	0.44
1:A:38:ASP:OD2	1:A:40:ASN:N	2.44	0.44
4:F:183:LEU:HD23	4:F:183:LEU:C	2.38	0.44
1:A:85:THR:HG22	1:A:222:TYR:CZ	2.53	0.44
1:A:76:PHE:HE1	1:A:78:ILE:HG13	1.82	0.44
3:E:207:TRP:N	7:E:303:ABU:HB2	2.32	0.44
2:D:121:GLN:HA	2:D:203:VAL:O	2.18	0.44
3:E:83:ILE:HG13	3:E:162:ASN:HB2	1.99	0.44
3:E:64:THR:OG1	3:E:66:LEU:HB2	2.17	0.44
2:B:59:ILE:HD13	2:B:68:ALA:HB3	2.00	0.44
3:E:14:LEU:HG	3:E:16:PRO:HD3	1.99	0.44
2:D:203:VAL:HG12	2:D:204:LEU:HD13	1.99	0.43
2:D:94:LEU:HG	2:D:210:ILE:HG22	1.99	0.43
3:E:45:PRO:CA	3:E:223:ILE:HD11	2.48	0.43
4:H:5:SER:CB	4:H:233:PHE:O	2.65	0.43
2:D:21:GLN:OE1	2:D:50:ARG:HD3	2.18	0.43
4:H:77:THR:HB	4:H:229:PHE:HZ	1.82	0.43
4:H:63:ALA:HB1	9:H:432:HOH:O	2.18	0.43
3:E:94:LEU:HB3	3:E:208:VAL:HG11	2.00	0.43
3:G:9:SER:HA	3:G:230:SER:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:ASP:OD1	1:C:12:LYS:NZ	2.49	0.43
2:B:50:ARG:HG2	2:B:213:SER:CB	2.47	0.43
2:D:5:SER:HA	2:D:233:PHE:O	2.18	0.43
1:A:207:TRP:CE2	2:D:16:PRO:HD2	2.53	0.43
4:F:21:GLN:OE1	4:F:50:ARG:HD2	2.18	0.43
3:G:42:VAL:HG21	9:G:408:HOH:O	2.18	0.43
1:A:149:SER:CB	9:A:402:HOH:O	2.66	0.43
2:B:210:ILE:HD12	2:B:231:TRP:CZ2	2.54	0.43
4:F:26:VAL:HA	4:F:31:VAL:O	2.19	0.43
3:E:205:PRO:HB2	7:E:303:ABU:CG	2.48	0.43
1:C:64:THR:HG22	1:C:66:VAL:H	1.83	0.43
1:A:121:GLN:HA	1:A:203:VAL:O	2.18	0.43
4:F:14:LEU:O	4:F:15:GLU:HB3	2.17	0.43
7:A:303:ABU:CA	2:D:17:ASN:ND2	2.75	0.43
3:E:246:SER:O	3:E:247:PHE:C	2.56	0.43
4:H:123:VAL:HG23	4:H:204:LEU:HD13	2.01	0.43
4:F:90:LEU:HD12	4:F:91:ALA:N	2.34	0.43
2:D:130:TYR:C	2:D:130:TYR:CD2	2.92	0.43
3:E:160:LEU:HD12	3:E:161:ALA:N	2.34	0.43
3:G:121:GLN:HA	3:G:148:ASN:HD21	1.84	0.43
4:F:51:ALA:O	4:F:211:GLY:HA3	2.19	0.43
2:D:9:SER:HA	2:D:230:SER:HB2	2.01	0.43
1:C:58:ASN:HB2	1:C:207:TRP:CH2	2.54	0.43
1:A:145:ILE:HG21	1:A:179:LEU:HD23	2.00	0.43
4:F:83:ILE:HD11	4:F:160:LEU:HD23	2.00	0.43
1:A:197:VAL:HG12	2:B:189:LYS:HD2	2.01	0.43
4:F:183:LEU:HD23	4:F:184:VAL:N	2.34	0.43
4:F:6:PHE:CZ	4:F:233:PHE:HB3	2.54	0.43
3:G:81:PRO:HD2	9:G:404:HOH:O	2.19	0.43
2:B:143:ILE:HG13	2:B:158:TRP:HB2	2.00	0.42
2:D:35:THR:CB	2:D:226:HIS:HD2	2.32	0.42
1:C:121:GLN:N	1:C:148:ASN:ND2	2.67	0.42
4:F:48:LEU:HD21	4:F:109:GLY:HA3	2.00	0.42
3:G:248:LEU:O	3:G:251:GLY:N	2.51	0.42
2:B:15:GLN:HA	2:B:16:PRO:HD3	1.68	0.42
4:F:52:THR:CG2	4:F:209:ARG:HB3	2.49	0.42
4:H:138:PRO:HD2	4:H:142:HIS:CE1	2.54	0.42
4:F:34:LEU:O	4:F:49:GLY:HA3	2.19	0.42
2:B:6:PHE:CE2	2:B:53:TYR:CD2	3.07	0.42
2:D:32:LEU:HG	2:D:34:LEU:HD13	2.02	0.42
2:D:191:SER:HB2	9:D:428:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:66:LEU:HD13	4:H:238:ALA:O	2.19	0.42
4:F:55:ALA:HA	4:F:56:PRO:HD2	1.79	0.42
3:G:185:TYR:HB2	3:G:190:THR:HG23	2.01	0.42
3:E:35:THR:CB	3:E:226:HIS:HD2	2.33	0.42
4:F:1:ALA:HA	3:G:9:SER:OG	2.19	0.42
1:C:80:ALA:HA	1:C:81:PRO:HD3	1.92	0.42
1:C:236:LYS:HZ2	1:C:236:LYS:HB3	1.84	0.42
1:A:125:VAL:HG13	1:A:170:ILE:HD13	2.01	0.42
3:E:85:THR:HB	3:E:222:LYS:HD3	2.00	0.42
2:D:77:THR:OG1	2:D:229:PHE:HZ	2.03	0.42
1:C:81:PRO:HD2	9:C:413:HOH:O	2.19	0.42
3:E:173:ASN:OD1	3:E:175:ALA:HB3	2.20	0.42
1:A:44:ASP:C	1:A:223:ILE:HD11	2.40	0.42
2:D:75:ARG:HD3	2:D:165:ALA:HB1	2.01	0.42
1:A:49:GLY:O	1:A:213:SER:HA	2.19	0.42
4:F:72:THR:HG21	4:F:92:PHE:CZ	2.55	0.42
3:G:95:ALA:HB1	3:G:96:PRO:CD	2.50	0.42
1:A:45:PRO:CB	1:A:46:LYS:HE2	2.31	0.42
3:G:83:ILE:N	3:G:83:ILE:HD12	2.33	0.42
2:B:180:VAL:HG22	2:B:195:SER:OG	2.20	0.42
1:C:64:THR:HG23	1:C:66:VAL:CG2	2.34	0.41
3:E:97:VAL:HG13	3:E:209:ARG:HH12	1.82	0.41
2:B:149:SER:HA	9:B:407:HOH:O	2.20	0.41
4:H:150:ILE:O	4:H:150:ILE:HG13	2.20	0.41
4:F:172:TYR:CE2	4:F:200:LEU:HD12	2.54	0.41
4:F:7:VAL:HB	4:F:232:SER:CB	2.50	0.41
2:B:183:LEU:HD23	2:B:183:LEU:C	2.41	0.41
1:C:210:ILE:O	1:C:210:ILE:HD12	2.21	0.41
1:C:183:LEU:HD23	1:C:183:LEU:C	2.41	0.41
1:C:180:VAL:HG11	8:D:304:GOL:H32	2.03	0.41
4:F:220:LYS:HE2	4:F:220:LYS:HA	2.03	0.41
1:A:207:TRP:CZ2	2:D:16:PRO:HD2	2.56	0.41
2:B:107:PHE:HE2	2:B:113:SER:HA	1.86	0.41
2:D:224:GLU:OE2	2:D:226:HIS:HE1	2.04	0.41
3:E:78:ILE:HD11	3:E:158:TRP:CH2	2.55	0.41
1:A:160:LEU:HD12	1:A:161:ALA:N	2.36	0.41
3:G:64:THR:OG1	3:G:66:LEU:CD2	2.69	0.41
2:D:150:ILE:HG13	2:D:150:ILE:O	2.20	0.41
4:H:50:ARG:HH21	4:H:110:LEU:HD23	1.86	0.41
1:A:94:LEU:O	1:A:122:THR:HA	2.21	0.41
2:B:78:ILE:HD11	2:B:90:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:ILE:HD13	2:D:162:ASN:ND2	2.35	0.41
2:D:83:ILE:HD11	2:D:160:LEU:CD2	2.46	0.41
3:E:248:LEU:O	3:E:250:GLY:N	2.54	0.41
4:F:233:PHE:CE2	4:F:235:SER:HB3	2.55	0.41
4:F:96:PRO:O	4:F:99:SER:HB3	2.21	0.41
3:E:184:VAL:CG1	4:F:178:LEU:HD21	2.51	0.41
4:H:76:PHE:CD1	4:H:90:LEU:HD21	2.56	0.41
3:G:80:ALA:HA	3:G:81:PRO:HD3	1.89	0.41
4:F:107:PHE:CE1	4:F:113:SER:HA	2.56	0.41
1:A:75:ARG:HD2	1:A:165:ALA:HB1	2.03	0.41
3:E:197:ILE:CD1	4:F:189:LYS:HD2	2.51	0.40
1:A:99:SER:HA	9:A:404:HOH:O	2.21	0.40
1:A:179:LEU:O	1:A:195:SER:HA	2.20	0.40
2:B:6:PHE:CE2	2:B:53:TYR:CG	3.09	0.40
3:G:188:SER:CB	3:G:190:THR:HG22	2.33	0.40
1:C:94:LEU:HA	1:C:210:ILE:HG22	2.03	0.40
1:C:87:ALA:HA	1:C:88:ASP:HA	1.95	0.40
2:B:161:ALA:HB3	2:B:185:TYR:CE1	2.56	0.40
2:B:1:THR:H2	1:C:9:SER:HB2	1.85	0.40
4:H:203:VAL:HG13	4:H:203:VAL:O	2.22	0.40
3:E:150:ILE:HG13	9:E:426:HOH:O	2.21	0.40
1:C:246:LEU:HD23	1:C:246:LEU:N	2.37	0.40
4:H:27:THR:HG1	4:H:29:ALA:HB3	1.87	0.40
4:F:77:THR:CB	4:F:229:PHE:HZ	2.35	0.40
1:A:75:ARG:HG3	1:A:229:PHE:HD2	1.87	0.40

There are no symmetry-related clashes.

## 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	245/255 (96%)	227 (93%)	15 (6%)	3 (1%)	16 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	245/255 (96%)	232 (95%)	11 (4%)	2 (1%)	24	41
2	B	237/239 (99%)	222 (94%)	12 (5%)	3 (1%)	15	26
2	D	237/239 (99%)	226 (95%)	10 (4%)	1 (0%)	39	61
3	E	245/251 (98%)	223 (91%)	17 (7%)	5 (2%)	9	15
3	G	245/251 (98%)	223 (91%)	19 (8%)	3 (1%)	16	29
4	F	237/239 (99%)	221 (93%)	16 (7%)	0	100	100
4	H	237/239 (99%)	219 (92%)	17 (7%)	1 (0%)	39	61
All	All	1928/1968 (98%)	1793 (93%)	117 (6%)	18 (1%)	21	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ILE
3	E	243	LYS
3	E	249	ASP
4	H	38	ASP
1	C	83	ILE
2	D	100	PRO
3	E	244	ASP
3	E	247	PHE
3	G	65	GLY
1	A	247	ASP
2	B	98	SER
2	B	149	SER
1	C	100	PRO
1	A	100	PRO
3	G	243	LYS
3	G	244	ASP
2	B	100	PRO
3	E	220	GLY

### 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	208/209 (100%)	176 (85%)	32 (15%)	3	6
1	C	208/209 (100%)	182 (88%)	26 (12%)	6	10
2	B	201/201 (100%)	180 (90%)	21 (10%)	9	16
2	D	201/201 (100%)	174 (87%)	27 (13%)	5	9
3	E	200/201 (100%)	172 (86%)	28 (14%)	4	8
3	G	200/201 (100%)	178 (89%)	22 (11%)	8	14
4	F	194/194 (100%)	168 (87%)	26 (13%)	5	9
4	H	194/194 (100%)	167 (86%)	27 (14%)	4	8
All	All	1606/1610 (100%)	1397 (87%)	209 (13%)	5	9

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	5	SER
1	A	9	SER
1	A	20	LYS
1	A	25	THR
1	A	32	LEU
1	A	38	ASP
1	A	44	ASP
1	A	46	LYS
1	A	75	ARG
1	A	90	LEU
1	A	97	VAL
1	A	102	LYS
1	A	116	PHE
1	A	123	VAL
1	A	125	VAL
1	A	129	THR
1	A	134	VAL
1	A	147	VAL
1	A	171	THR
1	A	174	SER
1	A	178	LEU
1	A	195	SER
1	A	197	VAL
1	A	198	VAL
1	A	200	LEU
1	A	210	ILE

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Mol	Chain	Res	Type
1	A	223	ILE
1	A	232	SER
1	A	238	SER
1	A	250	SER
1	A	253	VAL
2	B	20	LYS
2	B	25	THR
2	B	28	SER
2	B	35	THR
2	B	38	ASP
2	B	39	LYS
2	B	44	ASP
2	B	48	LEU
2	B	50	ARG
2	B	52	LEU
2	B	59	ILE
2	B	88	ASP
2	B	99	SER
2	B	151	LYS
2	B	153	ILE
2	B	171	THR
2	B	179	LEU
2	B	189	LYS
2	B	200	LEU
2	B	219	SER
2	B	225	THR
1	C	1	THR
1	C	19	LYS
1	C	20	LYS
1	C	25	THR
1	C	36	LYS
1	C	44	ASP
1	C	46	LYS
1	C	52	LEU
1	C	58	ASN
1	C	59	ILE
1	C	64	THR
1	C	83	ILE
1	C	90	LEU
1	C	97	VAL
1	C	98	SER
1	C	102	LYS

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Mol	Chain	Res	Type
1	C	110	LEU
1	C	115	VAL
1	C	118	SER
1	C	136	LEU
1	C	140	ASP
1	C	171	THR
1	C	198	VAL
1	C	200	LEU
1	C	201	LYS
1	C	252	LEU
2	D	9	SER
2	D	19	LYS
2	D	34	LEU
2	D	35	THR
2	D	44	ASP
2	D	46	LYS
2	D	52	LEU
2	D	55	SER
2	D	59	ILE
2	D	63	LYS
2	D	75	ARG
2	D	90	LEU
2	D	118	SER
2	D	119	SER
2	D	133	THR
2	D	134	VAL
2	D	140	ASP
2	D	153	ILE
2	D	171	THR
2	D	177	LYS
2	D	189	LYS
2	D	191	SER
2	D	200	LEU
2	D	201	LYS
2	D	204	LEU
2	D	236	LYS
2	D	239	PHE
3	E	5	SER
3	E	10	LYS
3	E	28	VAL
3	E	32	LEU
3	E	34	LEU

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Mol	Chain	Res	Type
3	E	35	THR
3	E	38	ASP
3	E	39	LYS
3	E	48	LEU
3	E	66	LEU
3	E	75	ARG
3	E	83	ILE
3	E	90	LEU
3	E	123	VAL
3	E	125	VAL
3	E	129	THR
3	E	133	THR
3	E	134	VAL
3	E	136	THR
3	E	147	VAL
3	E	171	THR
3	E	178	LEU
3	E	188	SER
3	E	189	LYS
3	E	198	VAL
3	E	208	VAL
3	E	210	VAL
3	E	223	ILE
4	F	5	SER
4	F	7	VAL
4	F	9	SER
4	F	18	LEU
4	F	38	ASP
4	F	39	SER
4	F	48	LEU
4	F	50	ARG
4	F	59	ILE
4	F	66	LEU
4	F	78	ILE
4	F	83	ILE
4	F	88	ASP
4	F	90	LEU
4	F	99	SER
4	F	115	VAL
4	F	118	THR
4	F	119	THR
4	F	136	THR

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Mol	Chain	Res	Type
4	F	153	ILE
4	F	171	THR
4	F	179	LEU
4	F	188	SER
4	F	191	SER
4	F	219	SER
4	F	220	LYS
3	G	19	ILE
3	G	25	LEU
3	G	27	THR
3	G	52	THR
3	G	58	ASN
3	G	59	ILE
3	G	66	LEU
3	G	75	ARG
3	G	83	ILE
3	G	88	ASP
3	G	102	ASP
3	G	110	LEU
3	G	167	LYS
3	G	171	THR
3	G	188	SER
3	G	190	THR
3	G	201	SER
3	G	236	LYS
3	G	237	LEU
3	G	242	THR
3	G	247	PHE
3	G	248	LEU
4	H	4	THR
4	H	10	LYS
4	H	14	LEU
4	H	25	LEU
4	H	26	VAL
4	H	34	LEU
4	H	35	THR
4	H	39	SER
4	H	48	LEU
4	H	52	THR
4	H	99	SER
4	H	103	SER
4	H	118	THR

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Mol	Chain	Res	Type
4	H	133	THR
4	H	134	VAL
4	H	151	SER
4	H	157	LYS
4	H	171	THR
4	H	188	SER
4	H	189	LYS
4	H	191	SER
4	H	197	ILE
4	H	202	SER
4	H	203	VAL
4	H	219	SER
4	H	220	LYS
4	H	237	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	14	ASN
1	A	15	GLN
1	A	17	ASN
1	A	58	ASN
1	A	82	ASN
1	A	148	ASN
1	A	226	HIS
2	B	15	GLN
2	B	58	ASN
2	B	132	ASN
2	B	148	ASN
2	B	226	HIS
1	C	148	ASN
1	C	226	HIS
2	D	17	ASN
2	D	33	GLN
2	D	58	ASN
2	D	226	HIS
3	E	21	GLN
3	E	33	GLN
3	E	58	ASN
3	E	132	ASN
3	E	148	ASN

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Mol	Chain	Res	Type
3	E	226	HIS
4	F	58	ASN
4	F	148	ASN
4	F	226	HIS
3	G	148	ASN
3	G	226	HIS
4	H	33	GLN
4	H	58	ASN
4	H	226	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 16 are monoatomic - leaving 9 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	$\# Z  > 2$
7	ABU	A	303	-	3,6,6	0.64	0	3,6,6	0.45	0
7	ABU	B	303	-	3,6,6	0.34	0	3,6,6	0.61	0
7	ABU	C	303	-	3,6,6	0.33	0	3,6,6	0.82	0
8	GOL	C	304	-	5,5,5	0.17	0	5,5,5	0.65	0
7	ABU	D	303	-	3,6,6	0.28	0	3,6,6	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	GOL	D	304	-	5,5,5	0.32	0	5,5,5	0.41	0
7	ABU	E	303	-	3,6,6	0.32	0	3,6,6	0.28	0
8	GOL	F	303	-	5,5,5	0.46	0	5,5,5	0.27	0
7	ABU	H	303	-	3,6,6	0.49	0	3,6,6	0.75	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
7	ABU	A	303	-	-	0/2/4/4	0/0/0/0
7	ABU	B	303	-	-	0/2/4/4	0/0/0/0
7	ABU	C	303	-	-	0/2/4/4	0/0/0/0
8	GOL	C	304	-	-	0/4/4/4	0/0/0/0
7	ABU	D	303	-	-	0/2/4/4	0/0/0/0
8	GOL	D	304	-	-	0/4/4/4	0/0/0/0
7	ABU	E	303	-	-	0/2/4/4	0/0/0/0
8	GOL	F	303	-	-	0/4/4/4	0/0/0/0
7	ABU	H	303	-	-	0/2/4/4	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.

9 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	303	ABU	3	0
7	B	303	ABU	7	0
7	C	303	ABU	10	0
8	C	304	GOL	1	0
7	D	303	ABU	7	0
8	D	304	GOL	3	0
7	E	303	ABU	9	0
8	F	303	GOL	1	0
7	H	303	ABU	8	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	249/255 (97%)	-0.03	13 (5%)	31 35	12, 24, 45, 65	1 (0%)
1	C	249/255 (97%)	0.12	15 (6%)	25 28	11, 26, 49, 77	0
2	B	239/239 (100%)	-0.15	4 (1%)	73 76	12, 24, 39, 62	1 (0%)
2	D	239/239 (100%)	-0.10	8 (3%)	50 55	10, 23, 40, 62	0
3	E	249/251 (99%)	0.10	12 (4%)	34 39	11, 24, 47, 114	0
3	G	249/251 (99%)	-0.04	9 (3%)	46 51	11, 24, 44, 100	0
4	F	239/239 (100%)	-0.12	3 (1%)	79 82	12, 24, 38, 54	0
4	H	239/239 (100%)	-0.20	3 (1%)	79 82	11, 22, 35, 49	0
All	All	1952/1968 (99%)	-0.05	67 (3%)	49 54	10, 24, 44, 114	2 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	242	THR	9.3
3	E	245	SER	7.2
3	G	245	SER	7.1
3	G	244	ASP	7.0
1	A	1	THR	5.5
1	C	1	THR	5.0
3	G	242	THR	5.0
3	G	243	LYS	5.0
1	A	250	SER	4.8
3	E	243	LYS	4.7
3	E	244	ASP	4.2
1	C	252	LEU	4.2
3	E	219	SER	4.2
1	C	253	VAL	4.1
1	C	118	SER	4.1
1	C	239	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	175	SER	3.9
3	E	218	ALA	3.7
3	E	115	VAL	3.7
3	G	250	GLY	3.6
1	C	133	THR	3.4
1	A	239	PHE	3.2
1	C	116	PHE	3.2
2	D	239	PHE	3.2
1	C	250	SER	3.1
2	D	1	THR	3.1
2	D	39	LYS	3.0
3	E	249	ASP	3.0
1	A	255	ASN	3.0
2	B	1	THR	3.0
1	A	247	ASP	2.9
4	F	118	THR	2.9
2	D	98	SER	2.9
4	F	1	ALA	2.9
1	C	175	SER	2.8
1	A	253	VAL	2.8
1	A	29	SER	2.8
1	A	119	SER	2.8
4	H	119	THR	2.8
3	E	246	SER	2.7
2	B	218	ALA	2.7
3	E	175	ALA	2.6
2	D	139	PRO	2.6
3	G	119	THR	2.6
2	B	98	SER	2.6
3	G	218	ALA	2.5
4	H	39	SER	2.5
1	C	46	LYS	2.4
2	B	175	SER	2.4
1	C	100	PRO	2.4
3	G	83	ILE	2.4
1	A	98	SER	2.4
1	A	175	SER	2.4
1	A	100	PRO	2.4
2	D	118	SER	2.4
1	C	97	VAL	2.3
3	G	246	SER	2.3
4	H	118	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	97	VAL	2.2
1	C	115	VAL	2.2
3	E	133	THR	2.2
2	D	100	PRO	2.2
1	C	255	ASN	2.2
3	E	46	SER	2.1
1	C	249	ALA	2.1
1	A	220	SER	2.1
4	F	98	ALA	2.1

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	ABU	E	303	7/7	0.90	0.30	9.46	23,25,27,27	7
7	ABU	A	303	7/7	0.85	0.30	5.42	14,16,17,18	7
7	ABU	D	303	7/7	0.86	0.28	5.13	25,29,36,42	7
8	GOL	F	303	6/6	0.91	0.17	4.35	23,27,28,28	6
7	ABU	B	303	7/7	0.87	0.27	4.16	15,16,17,19	7
7	ABU	H	303	7/7	0.88	0.26	3.67	15,17,19,20	7
7	ABU	C	303	7/7	0.94	0.20	1.21	19,21,21,23	7
8	GOL	D	304	6/6	0.92	0.15	1.10	25,26,26,27	6
8	GOL	C	304	6/6	0.87	0.21	0.71	30,32,34,35	6
5	CA	E	301	1/1	0.99	0.08	-1.88	31,31,31,31	0
6	MN	E	302	1/1	0.98	0.06	-2.10	35,35,35,35	0
5	CA	B	301	1/1	0.99	0.07	-2.30	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MN	A	302	1/1	0.98	0.04	-2.33	39,39,39,39	0
6	MN	C	302	1/1	1.00	0.04	-2.37	36,36,36,36	0
5	CA	A	301	1/1	1.00	0.04	-2.48	18,18,18,18	0
5	CA	C	301	1/1	0.98	0.05	-3.00	38,38,38,38	0
6	MN	H	302	1/1	0.98	0.04	-3.21	41,41,41,41	0
5	CA	H	301	1/1	0.98	0.05	-3.30	23,23,23,23	0
6	MN	G	302	1/1	0.99	0.02	-3.90	30,30,30,30	0
6	MN	B	302	1/1	0.99	0.04	-3.90	27,27,27,27	0
5	CA	G	301	1/1	0.99	0.03	-4.21	22,22,22,22	0
5	CA	F	301	1/1	0.97	0.04	-4.37	28,28,28,28	0
6	MN	F	302	1/1	1.00	0.01	-4.52	31,31,31,31	0
6	MN	D	302	1/1	0.98	0.03	-4.94	33,33,33,33	0
5	CA	D	301	1/1	0.99	0.04	-5.39	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.