



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:23 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 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/ValidationPDFNotes.html>

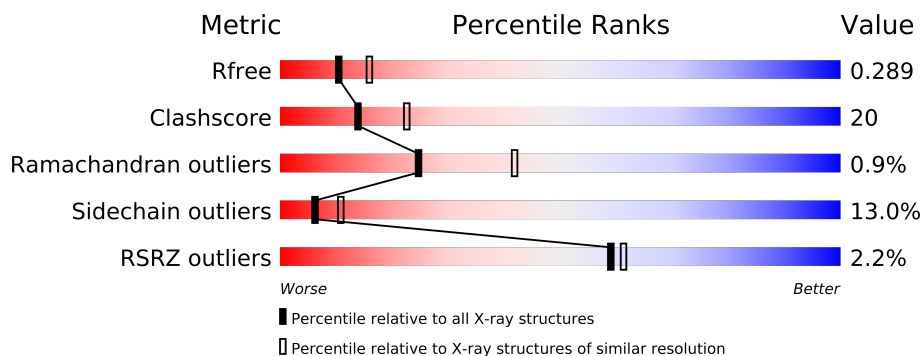
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	255	
1	C	255	
2	B	239	
2	D	239	
3	E	251	
3	G	251	
4	F	239	
4	H	239	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	ABU	A	303	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
7	ABU	B	303	-	X
7	ABU	D	303	-	X
7	ABU	E	303	-	X
7	ABU	H	303	-	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 hydrogen and 0 are deuterium.

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			

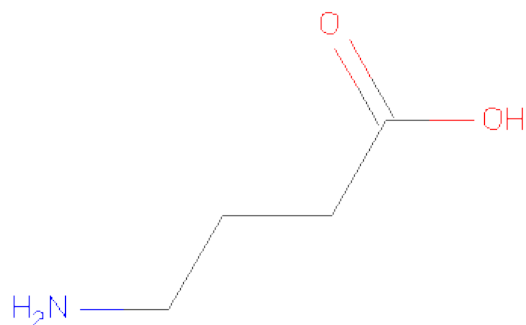
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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: C₄H₉NO₂).



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: C₃H₈O₃).



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		

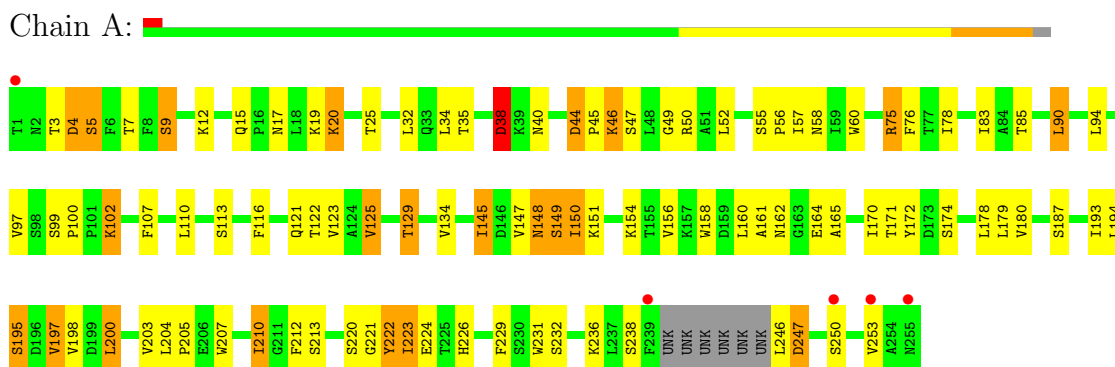
- Molecule 9 is water.

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		

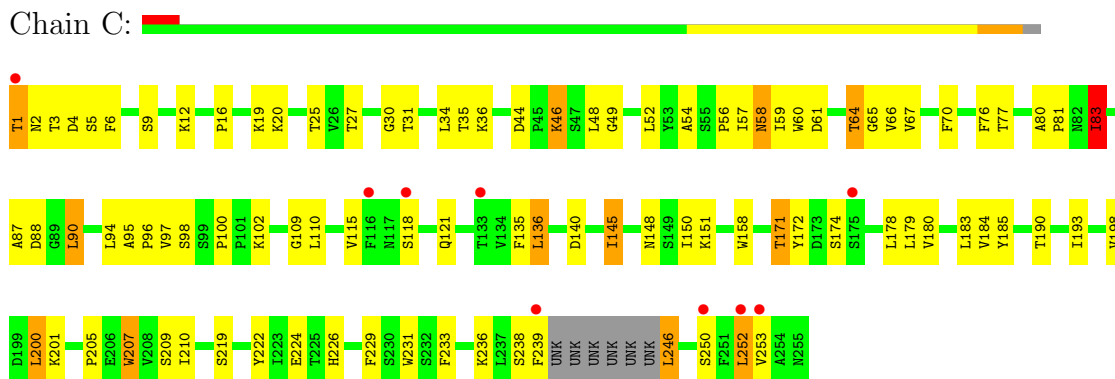
3 Residue-property plots

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.

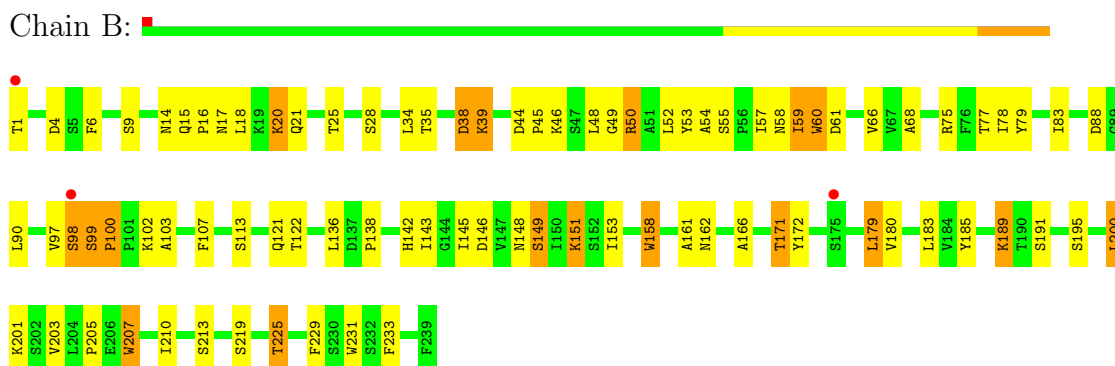
- Molecule 1: Lectin Alpha chain



- Molecule 1: Lectin Alpha chain

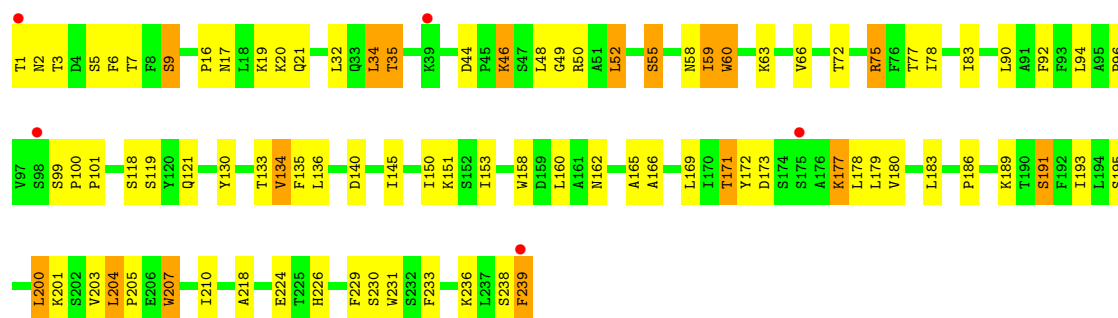


- Molecule 2: Lectin Beta Chain



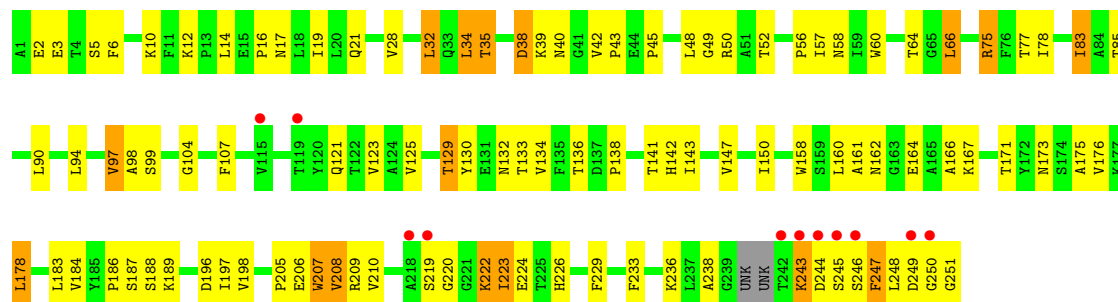
- Molecule 2: Lectin Beta Chain

Chain D:



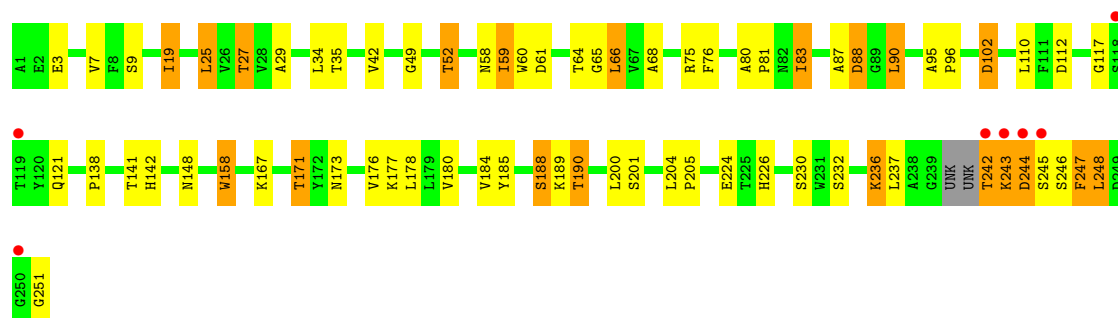
- Molecule 3: Seed lectin alpha chain

Chain E:



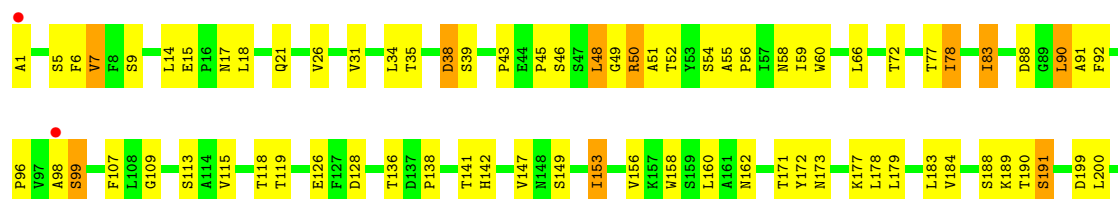
- Molecule 3: Seed lectin alpha chain

Chain G:



- Molecule 4: Seed lectin beta chain

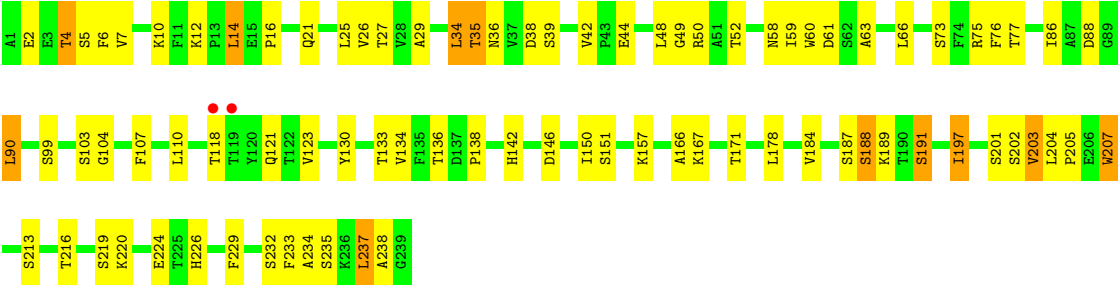
Chain F:





● Molecule 4: Seed lectin beta chain

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 95.6 (15.84-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.97 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.211 , 0.289 0.211 , 0.289	Depositor DCC
R_{free} test set	3641 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 16.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 72772 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15035	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	6	0	8	1	0
8	D	6	0	8	3	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (582) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:C:209:SER:HG	8:C:304:GOL:HO1	1.25	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	245/255 (96%)	227 (93%)	15 (6%)	3 (1%)	19	32
1	C	245/255 (96%)	232 (95%)	11 (4%)	2 (1%)	27	46
2	B	237/239 (99%)	222 (94%)	12 (5%)	3 (1%)	18	29
2	D	237/239 (99%)	226 (95%)	10 (4%)	1 (0%)	43	66
3	E	245/251 (98%)	223 (91%)	17 (7%)	5 (2%)	11	17
3	G	245/251 (98%)	223 (91%)	19 (8%)	3 (1%)	19	32
4	F	237/239 (99%)	221 (93%)	16 (7%)	0	100	100
4	H	237/239 (99%)	219 (92%)	17 (7%)	1 (0%)	43	66
All	All	1928/1968 (98%)	1793 (93%)	117 (6%)	18 (1%)	25	42

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%)	4	7
1	C	208/209 (100%)	182 (88%)	26 (12%)	7	12
2	B	201/201 (100%)	180 (90%)	21 (10%)	10	18
2	D	201/201 (100%)	174 (87%)	27 (13%)	6	10
3	E	200/201 (100%)	172 (86%)	28 (14%)	5	9
3	G	200/201 (100%)	178 (89%)	22 (11%)	9	16
4	F	194/194 (100%)	168 (87%)	26 (13%)	6	10
4	H	194/194 (100%)	167 (86%)	27 (14%)	5	9
All	All	1606/1610 (100%)	1397 (87%)	209 (13%)	6	11

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	6,6,6	0.53	0	6,6,6	1.86	2 (33%)
7	ABU	B	303	-	6,6,6	0.56	0	6,6,6	1.76	2 (33%)
7	ABU	C	303	-	6,6,6	1.04	1 (16%)	6,6,6	1.16	0
8	GOL	C	304	-	5,5,5	0.17	0	5,5,5	0.61	0
7	ABU	D	303	-	6,6,6	0.72	0	6,6,6	0.90	0
8	GOL	D	304	-	5,5,5	0.31	0	5,5,5	0.47	0
7	ABU	E	303	-	6,6,6	0.63	0	6,6,6	1.03	0
8	GOL	F	303	-	5,5,5	0.43	0	5,5,5	0.31	0
7	ABU	H	303	-	6,6,6	0.90	0	6,6,6	0.88	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	-	-	0/4/4/4	0/0/0/0
7	ABU	B	303	-	-	0/4/4/4	0/0/0/0
7	ABU	C	303	-	-	0/4/4/4	0/0/0/0
8	GOL	C	304	-	-	0/4/4/4	0/0/0/0
7	ABU	D	303	-	-	0/4/4/4	0/0/0/0
8	GOL	D	304	-	-	0/4/4/4	0/0/0/0
7	ABU	E	303	-	-	0/4/4/4	0/0/0/0
8	GOL	F	303	-	-	0/4/4/4	0/0/0/0
7	ABU	H	303	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	303	ABU	OE2-CD	-2.22	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	303	ABU	OE1-CD-CG	-3.49	111.02	123.03
7	B	303	ABU	OE2-CD-CG	2.92	124.52	114.22
7	B	303	ABU	OE1-CD-CG	-2.80	113.38	123.03
7	A	303	ABU	OE2-CD-CG	2.73	123.86	114.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	249/255 (97%)	-0.20	5 (2%) 62 64	12, 24, 45, 65	1 (0%)
1	C	249/255 (97%)	-0.07	9 (3%) 41 42	11, 26, 49, 77	0
2	B	239/239 (100%)	-0.28	3 (1%) 74 76	12, 24, 39, 62	1 (0%)
2	D	239/239 (100%)	-0.26	5 (2%) 60 63	10, 23, 40, 62	0
3	E	249/251 (99%)	-0.10	11 (4%) 33 34	11, 24, 47, 114	0
3	G	249/251 (99%)	-0.20	7 (2%) 50 53	11, 24, 44, 100	0
4	F	239/239 (100%)	-0.27	2 (0%) 83 84	12, 24, 38, 54	0
4	H	239/239 (100%)	-0.31	2 (0%) 83 84	11, 22, 35, 49	0
All	All	1952/1968 (99%)	-0.21	44 (2%) 59 60	10, 24, 44, 114	2 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	242	THR	6.2
3	G	245	SER	5.6
3	E	245	SER	5.3
3	G	244	ASP	5.1
1	A	1	THR	5.0
3	G	242	THR	4.2
3	E	243	LYS	4.1
3	G	243	LYS	4.0
1	C	239	PHE	4.0
1	A	250	SER	3.7
1	C	1	THR	3.7
3	G	250	GLY	3.7
1	C	253	VAL	3.6
1	C	252	LEU	3.3
2	D	175	SER	3.2
2	D	1	THR	3.1

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Mol	Chain	Res	Type	RSRZ
3	E	219	SER	2.9
3	E	244	ASP	2.9
1	C	133	THR	2.9
1	A	239	PHE	2.8
2	B	1	THR	2.8
4	H	118	THR	2.8
2	D	98	SER	2.7
3	E	218	ALA	2.5
1	A	253	VAL	2.5
1	C	116	PHE	2.5
3	E	115	VAL	2.5
2	D	239	PHE	2.5
4	F	1	ALA	2.5
1	C	250	SER	2.5
3	E	246	SER	2.5
3	G	118	SER	2.5
1	C	118	SER	2.3
1	C	175	SER	2.3
3	E	249	ASP	2.3
3	E	250	GLY	2.3
2	B	175	SER	2.2
1	A	255	ASN	2.2
4	F	98	ALA	2.2
3	E	119	THR	2.1
2	B	98	SER	2.1
2	D	39	LYS	2.1
3	G	119	THR	2.1
4	H	119	THR	2.0

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

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	ABU	E	303	7/7	0.27	5.24	23,25,27,27	7
7	ABU	D	303	7/7	0.25	5.20	25,29,36,42	7
8	GOL	F	303	6/6	0.16	4.72	23,27,28,28	6
7	ABU	A	303	7/7	0.26	4.58	14,16,17,18	7
7	ABU	H	303	7/7	0.23	3.24	15,17,19,20	7
7	ABU	B	303	7/7	0.24	3.18	15,16,17,19	7
8	GOL	D	304	6/6	0.16	1.56	25,26,26,27	6
8	GOL	C	304	6/6	0.22	1.31	30,32,34,35	6
7	ABU	C	303	7/7	0.16	1.01	19,21,21,23	7
5	CA	E	301	1/1	0.07	-1.85	31,31,31,31	0
5	CA	B	301	1/1	0.06	-2.03	23,23,23,23	0
5	CA	A	301	1/1	0.04	-2.31	18,18,18,18	0
6	MN	A	302	1/1	0.04	-2.54	39,39,39,39	0
5	CA	H	301	1/1	0.05	-2.83	23,23,23,23	0
5	CA	C	301	1/1	0.03	-3.00	38,38,38,38	0
6	MN	C	302	1/1	0.01	-3.19	36,36,36,36	0
6	MN	E	302	1/1	0.03	-3.19	35,35,35,35	0
6	MN	H	302	1/1	0.04	-3.29	41,41,41,41	0
5	CA	G	301	1/1	0.03	-3.36	22,22,22,22	0
6	MN	G	302	1/1	0.02	-3.58	30,30,30,30	0
6	MN	B	302	1/1	0.03	-3.76	27,27,27,27	0
5	CA	D	301	1/1	0.04	-4.00	25,25,25,25	0
6	MN	F	302	1/1	0.02	-4.15	31,31,31,31	0
5	CA	F	301	1/1	0.04	-4.15	28,28,28,28	0
6	MN	D	302	1/1	0.03	-5.75	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.