



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:03 AM GMT

PDB ID : 2P6G
Title : Crystal structures of *Saccharomyces cerevisiae* N-myristoyltransferase with bound myristoyl-CoA and inhibitors
Authors : Wu, J.; Ding, J.
Deposited on : 2007-03-18
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

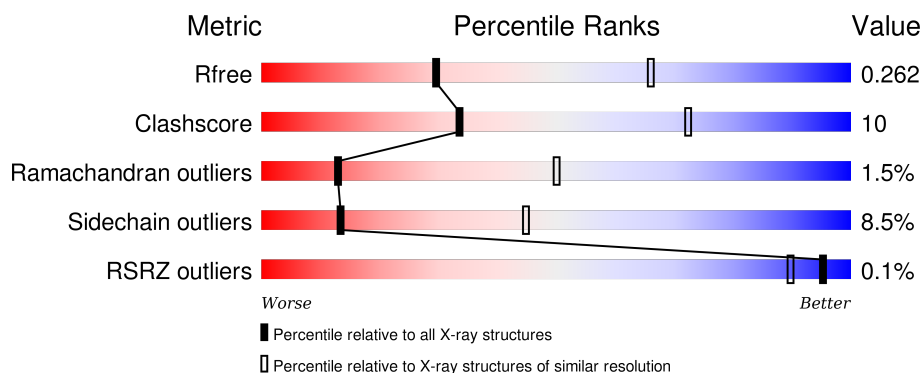
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	455	 71% 22% . .
1	B	455	 69% 23% . .
1	C	455	 66% 26% . .
1	D	455	 70% 23% . .
1	E	455	 68% 23% . .

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Mol	Chain	Length	Quality of chain
1	F	455	 <div>69% 22%</div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MYA	A	601	X	-	-	-
2	MYA	B	602	X	-	-	-
2	MYA	C	603	X	-	-	-
2	MYA	D	604	X	-	-	-
2	MYA	E	605	X	-	-	-
2	MYA	F	606	X	-	-	-
3	3LP	C	703	-	-	-	X
3	3LP	F	706	-	-	X	X

2 Entry composition [i](#)

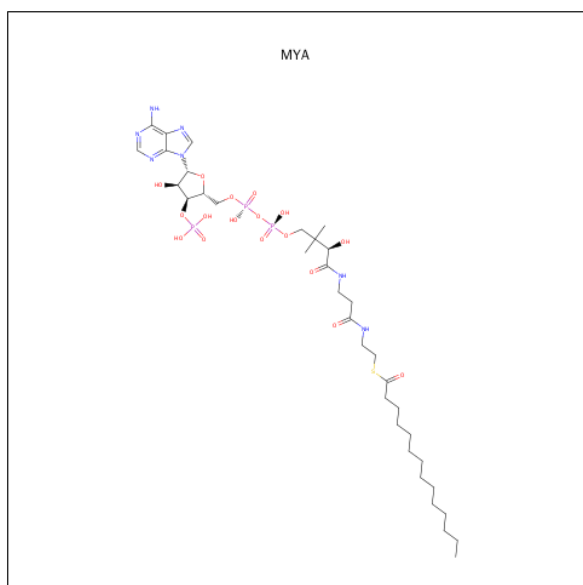
There are 3 unique types of molecules in this entry. The entry contains 21848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycylpeptide N-tetradecanoyltransferase.

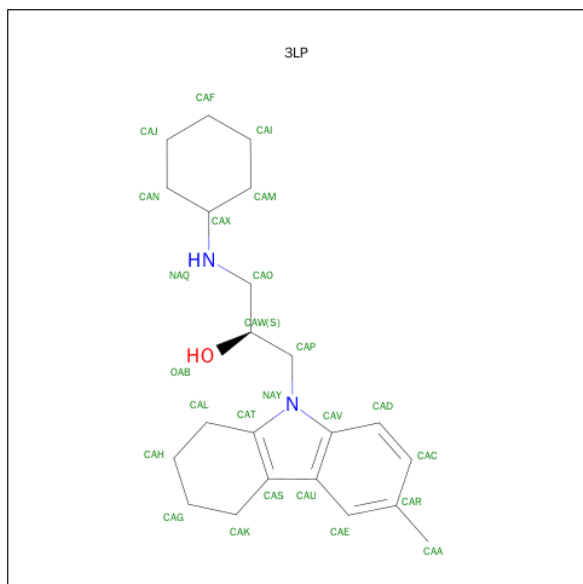
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			
1	B	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			
1	C	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			
1	D	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			
1	E	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			
1	F	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			

- Molecule 2 is TETRADECANOYL-COA (three-letter code: MYA) (formula: $C_{35}H_{62}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 3 is 1-(CYCLOHEXYLAMINO)-3-(6-METHYL-3,4-DIHYDRO-1H-CARBAZOL-9(2H)-YL)PROPAN-2-OL (three-letter code: 3LP) (formula: C₂₂H₃₂N₂O).

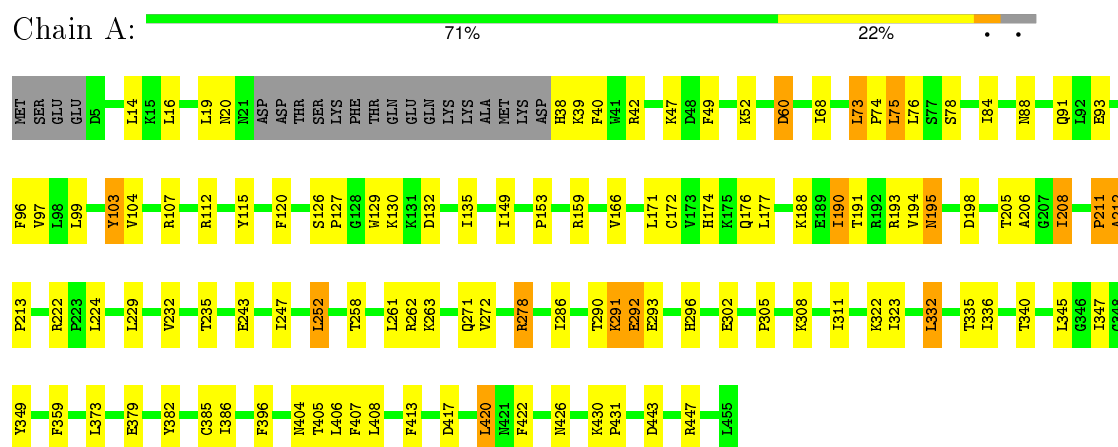


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			25	22	2	1		
3	F	1	Total	C	N	O	0	0
			25	22	2	1		

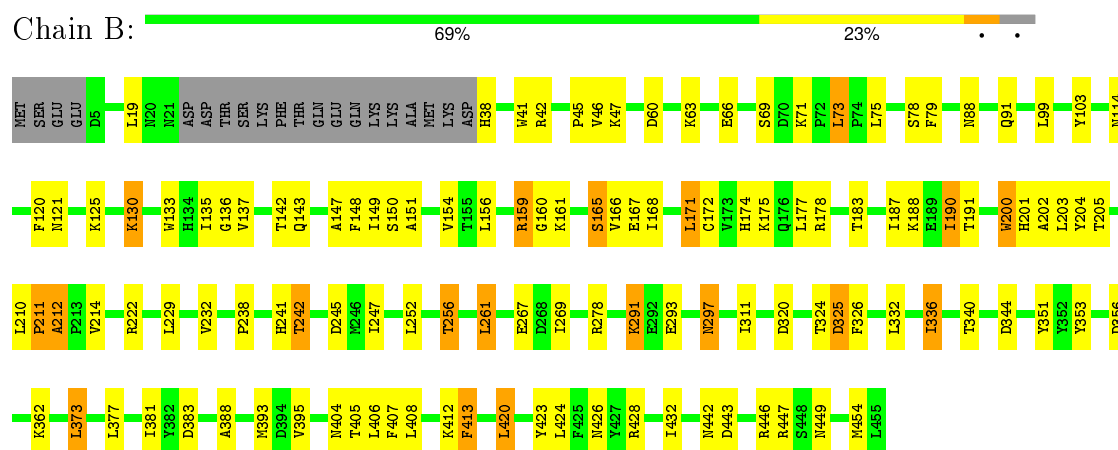
3 Residue-property plots

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.

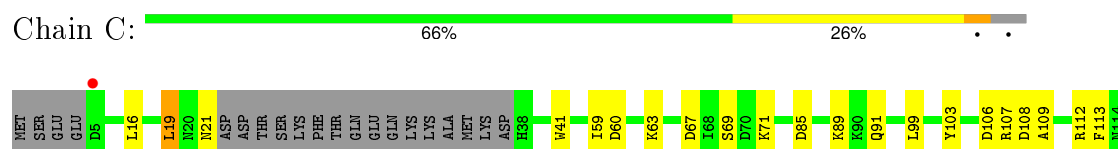
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

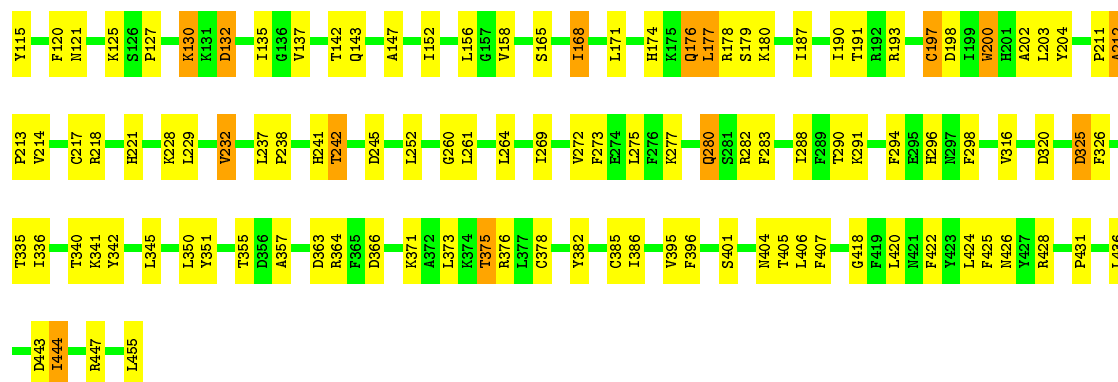


• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

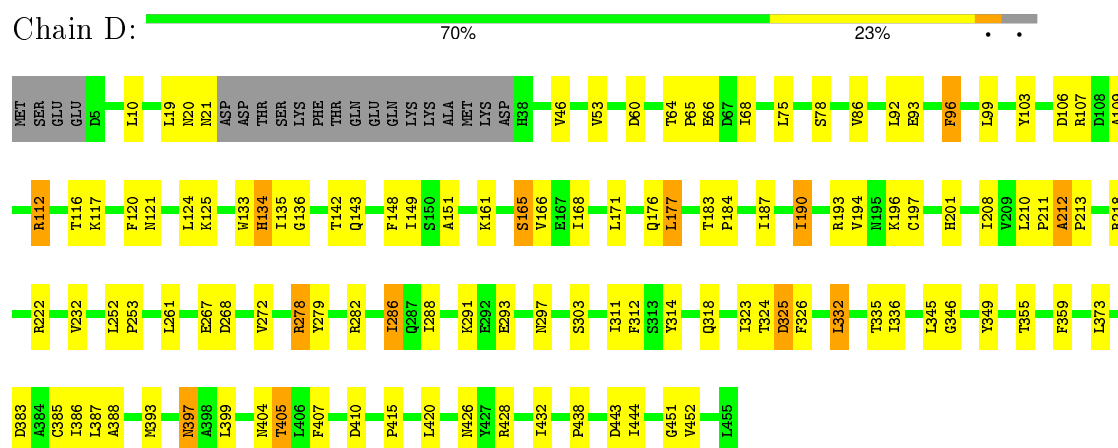


• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

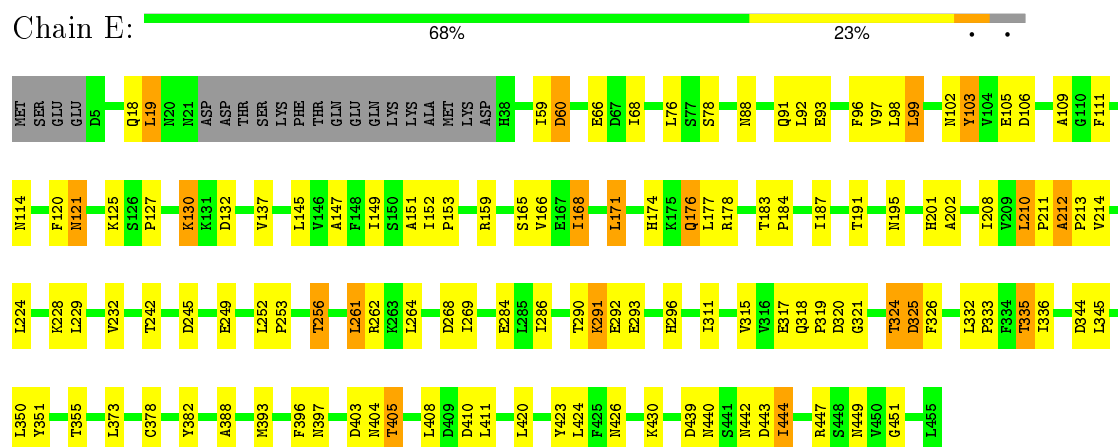




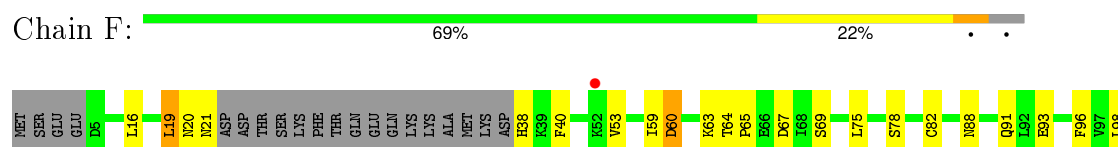
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



D356	L229	L99	D357	V232	Y103	D358	L237	Y104	E105	R364	D239	P238	R112	K117	N121	K130	L145	F148	I152	L156	G157	V158	R159	G160	S165	L171	H174	K175	Q176	L177	K180	T183	K188	E189	I190	V194	W200	L203	Y204	T205	P211	A212	Y219	R222	P223	L224																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
D356	D357	D358	R364	K371	A372	L373	K374	T375	C378	Y382	C385	I386	N392	F396	Q402	D403	N404	T405	L406	F407	K412	D417	G418	F419	L420	N421	N426	Y427	R428	N442	G451	V452	L455																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.85Å 151.30Å 134.19Å 90.00° 107.64° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 14.98 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-3.00) 97.7 (14.98-2.99)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.260 , 0.318 0.262 , 0.262	Depositor DCC
R_{free} test set	3526 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 16.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	4 of 70172 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	21848	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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 43.51 % 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 1.7446e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MYA, 3LP

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	0.34	0/3658	0.54	0/4946
1	B	0.34	0/3658	0.53	0/4946
1	C	0.34	0/3658	0.52	0/4946
1	D	0.34	0/3658	0.52	0/4946
1	E	0.34	0/3658	0.53	0/4946
1	F	0.34	0/3658	0.53	0/4946
All	All	0.34	0/21948	0.53	0/29676

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3570	0	3569	68	0
1	B	3570	0	3569	79	0
1	C	3570	0	3569	75	0
1	D	3570	0	3569	70	0
1	E	3570	0	3569	80	0
1	F	3570	0	3569	81	0
2	A	63	0	58	3	0
2	B	63	0	58	11	0
2	C	63	0	58	5	0
2	D	63	0	58	3	0
2	E	63	0	58	9	0
2	F	63	0	58	4	0
3	C	25	0	32	4	0
3	F	25	0	32	10	0
All	All	21848	0	21826	447	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 10.

All (447) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ARG:HH11	1:D:112:ARG:HG2	1.09	1.11
1:D:212:ALA:H	1:D:213:PRO:HD3	1.18	1.02
1:D:60:ASP:H	1:D:426:ASN:HD21	1.21	0.87
1:A:127:PRO:HG2	1:A:293:GLU:HA	1.56	0.85
1:D:212:ALA:N	1:D:213:PRO:HD3	1.89	0.85
1:F:418:GLY:HA3	3:F:706:3LP:HAH2	1.59	0.85
1:A:159:ARG:NH2	1:A:430:LYS:O	2.10	0.84
1:C:60:ASP:H	1:C:426:ASN:HD21	1.28	0.82
1:D:212:ALA:H	1:D:213:PRO:CD	1.94	0.81
1:C:198:ASP:HA	1:C:200:TRP:HZ3	1.47	0.80
1:E:212:ALA:H	1:E:213:PRO:CD	1.95	0.80
1:D:112:ARG:NH1	1:D:112:ARG:HG2	1.88	0.80
1:E:350:LEU:HB2	1:E:396:PHE:HE2	1.48	0.78
1:F:222:ARG:HH21	1:F:412:LYS:HG3	1.47	0.77
1:A:336:ILE:HD11	1:A:345:LEU:HB2	1.66	0.77
1:B:168:ILE:HG13	2:B:602:MYA:HAMA	1.67	0.77
1:A:127:PRO:HD3	1:A:296:HIS:CD2	2.20	0.76
1:D:187:ILE:HD12	2:D:604:MYA:H7M	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:HG21	1:A:112:ARG:HA	1.65	0.75
1:A:305:PRO:HG2	1:A:308:LYS:HG3	1.67	0.75
1:D:218:ARG:HH21	1:D:415:PRO:HB2	1.52	0.75
1:A:191:THR:HA	2:A:601:MYA:HDM	1.70	0.74
1:C:198:ASP:HA	1:C:200:TRP:CZ3	2.22	0.73
1:D:405:THR:HG21	1:D:443:ASP:O	1.87	0.73
1:A:47:LYS:HB3	1:A:212:ALA:HB1	1.71	0.72
1:B:404:ASN:HA	1:B:407:PHE:CE2	2.24	0.72
1:A:99:LEU:O	1:A:103:TYR:HB2	1.90	0.71
1:B:60:ASP:H	1:B:426:ASN:HD21	1.37	0.71
1:D:107:ARG:HH22	1:F:21:ASN:HB3	1.55	0.71
2:C:603:MYA:HN8	2:C:603:MYA:H13B	1.56	0.70
1:D:112:ARG:HH11	1:D:112:ARG:CG	1.96	0.70
1:E:318:GLN:HB3	1:E:319:PRO:HD2	1.73	0.69
1:E:165:SER:HB3	1:E:201:HIS:HB2	1.73	0.69
1:B:242:THR:HB	1:B:245:ASP:H	1.57	0.69
1:B:222:ARG:HH21	1:B:412:LYS:HG3	1.56	0.68
1:C:60:ASP:N	1:C:426:ASN:HD21	1.91	0.68
1:E:290:THR:H	1:E:293:GLU:HG2	1.58	0.68
1:C:336:ILE:HD11	1:C:345:LEU:HB2	1.75	0.68
1:E:212:ALA:H	1:E:213:PRO:HD2	1.57	0.68
1:F:418:GLY:H	3:F:706:3LP:HAG2	1.58	0.67
1:E:168:ILE:HG21	2:E:605:MYA:H7M	1.77	0.67
1:B:405:THR:HG23	1:B:442:ASN:HB3	1.75	0.67
1:D:176:GLN:HG2	1:F:19:LEU:HB2	1.76	0.67
1:F:156:LEU:HD11	1:F:203:LEU:HB2	1.77	0.67
1:F:405:THR:HG23	1:F:442:ASN:HB3	1.75	0.67
1:F:219:TYR:CD1	3:F:706:3LP:HAL1	2.31	0.66
1:E:403:ASP:OD1	1:E:447:ARG:HD2	1.95	0.66
1:E:262:ARG:HH21	1:E:317:GLU:HB2	1.61	0.66
1:A:47:LYS:O	1:A:212:ALA:HB2	1.96	0.66
1:B:151:ALA:HB2	1:B:190:ILE:HD11	1.77	0.66
1:F:60:ASP:H	1:F:426:ASN:HD21	1.42	0.65
1:C:156:LEU:HG	1:C:165:SER:OG	1.96	0.65
1:E:159:ARG:NH2	1:E:430:LYS:O	2.30	0.65
1:B:135:ILE:HD12	1:B:190:ILE:HG12	1.77	0.65
1:F:418:GLY:HA3	3:F:706:3LP:CAH	2.27	0.64
1:A:205:THR:HB	1:A:420:LEU:HD21	1.79	0.64
1:F:104:VAL:HG21	1:F:112:ARG:HA	1.79	0.64
1:D:151:ALA:HB2	1:D:190:ILE:HD11	1.80	0.64
1:C:371:LYS:O	1:C:375:THR:HG22	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:THR:HB	1:A:420:LEU:CD2	2.28	0.64
1:E:350:LEU:HB2	1:E:396:PHE:CE2	2.31	0.63
1:B:137:VAL:HB	1:B:147:ALA:HB3	1.80	0.63
1:E:111:PHE:HA	1:E:335:THR:O	1.99	0.62
1:B:63:LYS:HB2	1:B:200:TRP:CZ2	2.34	0.62
1:B:191:THR:HA	2:B:602:MYA:HDM	1.82	0.62
1:D:107:ARG:NH2	1:F:21:ASN:HB3	2.14	0.62
1:B:232:VAL:CG1	1:B:336:ILE:HG12	2.30	0.62
1:D:325:ASP:HB3	1:D:355:THR:HA	1.81	0.62
1:C:237:LEU:HD21	1:C:241:HIS:O	2.00	0.62
1:E:405:THR:HG21	1:E:443:ASP:O	2.00	0.61
1:F:382:TYR:O	1:F:386:ILE:HG12	2.00	0.61
1:B:47:LYS:HD2	1:B:212:ALA:HB1	1.83	0.61
1:C:405:THR:HG21	1:C:443:ASP:O	2.01	0.61
1:C:242:THR:HB	1:C:245:ASP:H	1.65	0.61
1:A:229:LEU:HB3	1:A:235:THR:HG22	1.83	0.61
1:F:117:LYS:O	1:F:121:ASN:HB2	2.01	0.60
1:B:408:LEU:O	1:B:413:PHE:HB2	2.00	0.60
1:D:60:ASP:H	1:D:426:ASN:ND2	1.95	0.60
1:C:121:ASN:O	1:C:125:LYS:HB2	2.02	0.60
1:C:418:GLY:HA3	3:C:703:3LP:HAH2	1.83	0.60
1:A:88:ASN:HD22	1:A:91:GLN:H	1.48	0.60
1:B:38:HIS:N	1:B:42:ARG:HH21	2.00	0.59
1:D:121:ASN:O	1:D:125:LYS:HB2	2.02	0.59
1:E:325:ASP:HB3	1:E:355:THR:HA	1.83	0.59
1:E:102:ASN:O	1:E:178:ARG:NH2	2.35	0.59
1:B:130:LYS:HE3	1:F:322:LYS:HB2	1.85	0.59
1:B:183:THR:O	1:B:187:ILE:HG12	2.02	0.59
1:E:60:ASP:H	1:E:426:ASN:HD21	1.49	0.59
1:C:214:VAL:HG21	1:C:424:LEU:HD12	1.84	0.58
1:B:205:THR:CG2	1:B:454:MET:HG3	2.33	0.58
1:A:107:ARG:HH22	1:C:21:ASN:C	2.05	0.58
1:D:252:LEU:HD21	1:D:385:CYS:HB3	1.85	0.58
1:F:177:LEU:HB2	1:F:180:LYS:HD2	1.84	0.58
1:A:135:ILE:HD11	1:A:193:ARG:HD2	1.85	0.58
1:C:191:THR:HA	2:C:603:MYA:HDM	1.86	0.58
1:B:174:HIS:HB3	1:B:177:LEU:CD2	2.33	0.58
1:C:168:ILE:HG22	1:C:204:TYR:HB3	1.85	0.58
1:C:217:CYS:HG	1:C:422:PHE:HE1	1.52	0.58
1:D:99:LEU:HD12	1:D:120:PHE:HZ	1.68	0.58
1:A:60:ASP:H	1:A:426:ASN:HD21	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:LEU:HD11	1:E:177:LEU:HD22	1.86	0.58
1:B:432:ILE:HG23	1:B:449:ASN:HB2	1.85	0.58
1:C:41:TRP:HB3	1:C:211:PRO:HG2	1.86	0.58
1:E:191:THR:HA	2:E:605:MYA:HDM	1.84	0.58
1:D:165:SER:HB3	1:D:201:HIS:HB2	1.85	0.57
1:B:256:THR:HG21	1:B:261:LEU:HD12	1.86	0.57
1:E:284:GLU:H	1:E:449:ASN:HB3	1.67	0.57
1:C:187:ILE:HG23	2:C:603:MYA:H9M	1.86	0.57
1:B:232:VAL:HG11	1:B:336:ILE:HG12	1.86	0.57
1:D:96:PHE:HE2	1:D:117:LYS:HB3	1.70	0.57
1:A:406:LEU:HG	1:A:447:ARG:HD3	1.86	0.57
1:B:41:TRP:HB3	1:B:211:PRO:HG2	1.87	0.56
1:C:455:LEU:O	3:C:703:3LP:HA12	2.05	0.56
1:F:252:LEU:HG	1:F:386:ILE:HD13	1.86	0.56
1:C:130:LYS:HG3	1:C:132:ASP:HB2	1.87	0.56
1:F:404:ASN:HA	1:F:407:PHE:CE2	2.41	0.56
1:F:174:HIS:HD2	1:F:176:GLN:HB3	1.71	0.56
1:C:187:ILE:HG12	2:C:603:MYA:H7MA	1.87	0.56
1:B:159:ARG:O	1:B:161:LYS:N	2.31	0.56
1:A:47:LYS:HB3	1:A:212:ALA:CB	2.35	0.55
1:F:38:HIS:HA	2:F:606:MYA:P3X	2.46	0.55
1:E:210:LEU:O	1:E:423:TYR:HE2	1.89	0.55
1:F:156:LEU:HG	1:F:165:SER:OG	2.06	0.55
1:E:60:ASP:H	1:E:426:ASN:ND2	2.04	0.55
1:F:315:VAL:HG22	1:F:323:ILE:HG23	1.89	0.55
1:C:378:CYS:O	1:C:382:TYR:HB2	2.07	0.55
1:D:293:GLU:O	1:D:297:ASN:HB2	2.07	0.55
1:B:149:ILE:HD12	1:B:171:LEU:HG	1.88	0.55
1:D:171:LEU:HD12	2:D:604:MYA:H5MA	1.88	0.55
1:E:183:THR:O	1:E:187:ILE:HG12	2.06	0.55
1:A:104:VAL:CG2	1:A:112:ARG:HA	2.37	0.55
1:A:60:ASP:H	1:A:426:ASN:ND2	2.05	0.55
1:B:151:ALA:HB2	1:B:190:ILE:CD1	2.37	0.54
1:C:404:ASN:HA	1:C:407:PHE:CE2	2.42	0.54
1:F:98:LEU:HD22	1:F:145:LEU:HG	1.89	0.54
1:D:93:GLU:HA	1:D:96:PHE:CE2	2.42	0.54
1:F:286:ILE:HG22	1:F:451:GLY:HA3	1.89	0.54
1:D:272:VAL:HG22	1:D:323:ILE:HG21	1.89	0.54
1:B:174:HIS:HB3	1:B:177:LEU:HD21	1.88	0.54
1:A:408:LEU:O	1:A:413:PHE:HB2	2.07	0.54
1:E:106:ASP:HB3	1:E:109:ALA:HB2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:THR:O	1:D:187:ILE:HG12	2.08	0.53
1:A:405:THR:HG21	1:A:443:ASP:O	2.08	0.53
1:D:405:THR:CG2	1:D:444:ILE:HA	2.38	0.53
1:F:305:PRO:HG2	1:F:308:LYS:HG3	1.89	0.53
1:E:212:ALA:HB3	1:E:423:TYR:HD2	1.73	0.53
1:E:232:VAL:O	1:E:232:VAL:HG12	2.09	0.53
1:A:126:SER:O	1:A:129:TRP:HD1	1.91	0.53
1:F:418:GLY:N	3:F:706:3LP:CAG	2.72	0.53
2:E:605:MYA:H13	2:E:605:MYA:N7A	2.23	0.53
1:B:147:ALA:HA	1:B:172:CYS:O	2.09	0.53
1:A:404:ASN:HA	1:A:407:PHE:CE2	2.43	0.53
1:C:63:LYS:HB3	1:C:67:ASP:HB2	1.91	0.53
1:F:222:ARG:NH2	1:F:412:LYS:HG3	2.21	0.53
1:F:60:ASP:H	1:F:426:ASN:ND2	2.06	0.53
1:B:204:TYR:CD2	2:B:602:MYA:H6MA	2.44	0.52
1:F:20:ASN:HD22	1:F:417:ASP:HB2	1.73	0.52
1:C:252:LEU:HD21	1:C:385:CYS:HB3	1.92	0.52
1:D:253:PRO:HD2	1:D:386:ILE:HG12	1.89	0.52
1:E:378:CYS:HA	1:E:411:LEU:HD11	1.92	0.52
1:B:238:PRO:HB2	1:B:241:HIS:HD2	1.73	0.52
1:B:63:LYS:HB2	1:B:200:TRP:HZ2	1.74	0.52
1:E:149:ILE:HD12	1:E:171:LEU:HG	1.91	0.52
1:B:121:ASN:O	1:B:125:LYS:HB2	2.10	0.52
1:E:211:PRO:O	1:E:212:ALA:HB2	2.09	0.52
1:C:238:PRO:HB2	1:C:241:HIS:HD2	1.75	0.52
1:C:325:ASP:HB3	1:C:355:THR:HA	1.91	0.52
1:A:84:ILE:HG23	1:A:91:GLN:HB3	1.91	0.52
1:F:418:GLY:H	3:F:706:3LP:CAG	2.22	0.51
1:E:93:GLU:O	1:E:97:VAL:HG23	2.09	0.51
1:D:232:VAL:O	1:D:232:VAL:HG12	2.10	0.51
1:A:176:GLN:HB3	1:C:19:LEU:HD12	1.93	0.51
1:F:211:PRO:O	1:F:212:ALA:HB3	2.11	0.51
1:E:174:HIS:HB3	1:E:177:LEU:CD2	2.40	0.51
1:B:214:VAL:HG21	1:B:424:LEU:HD12	1.92	0.51
1:F:262:ARG:HH21	1:F:317:GLU:HB2	1.76	0.51
1:D:112:ARG:CG	1:D:112:ARG:NH1	2.62	0.51
1:F:158:VAL:C	1:F:160:GLY:H	2.14	0.51
1:F:63:LYS:HB2	1:F:200:TRP:HZ2	1.76	0.50
1:C:444:ILE:H	1:C:444:ILE:HD13	1.76	0.50
1:E:174:HIS:CD2	1:E:176:GLN:H	2.29	0.50
1:A:271:GLN:OE1	1:A:322:LYS:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ILE:HG23	2:B:602:MYA:H9M	1.93	0.50
1:A:405:THR:HG21	1:A:443:ASP:C	2.32	0.50
1:D:106:ASP:HB3	1:D:109:ALA:HB2	1.94	0.50
1:F:418:GLY:N	3:F:706:3LP:HAG2	2.26	0.50
1:B:99:LEU:O	1:B:103:TYR:HB2	2.11	0.50
1:C:273:PHE:CE2	1:C:277:LYS:HG3	2.47	0.50
1:C:197:CYS:O	1:C:198:ASP:HB2	2.11	0.49
1:B:60:ASP:H	1:B:426:ASN:ND2	2.09	0.49
1:F:171:LEU:HB2	2:F:606:MYA:H3M	1.95	0.49
1:F:63:LYS:HB3	1:F:67:ASP:HB2	1.94	0.49
1:C:59:ILE:HG23	1:C:428:ARG:NH2	2.26	0.49
1:C:294:PHE:O	1:C:298:PHE:HD1	1.95	0.49
1:A:38:HIS:HA	2:A:601:MYA:P3X	2.52	0.49
2:F:606:MYA:H3MA	2:F:606:MYA:N1A	2.27	0.49
1:C:202:ALA:HB3	1:C:425:PHE:HB3	1.94	0.49
1:B:88:ASN:HB3	1:B:91:GLN:HB2	1.94	0.49
1:D:183:THR:HB	1:D:184:PRO:HD3	1.94	0.49
1:C:156:LEU:HD11	1:C:203:LEU:HB2	1.95	0.49
1:B:205:THR:HG21	1:B:454:MET:HG3	1.95	0.49
1:C:228:LYS:O	1:C:232:VAL:HB	2.12	0.49
1:B:142:THR:O	1:B:143:GLN:HB2	2.13	0.49
1:F:171:LEU:HD11	1:F:183:THR:HG23	1.94	0.49
1:A:126:SER:O	1:A:129:TRP:CD1	2.65	0.49
1:C:115:TYR:OH	3:C:703:3LP:HAF1	2.12	0.49
1:B:205:THR:HG23	1:B:454:MET:HG3	1.94	0.49
1:A:252:LEU:HD21	1:A:385:CYS:HB3	1.94	0.49
1:A:258:THR:HG21	1:A:379:GLU:HB3	1.95	0.49
1:D:318:GLN:HG2	1:D:324:THR:OG1	2.11	0.49
1:E:59:ILE:H	1:E:426:ASN:ND2	2.11	0.48
1:D:286:ILE:HG22	1:D:451:GLY:HA3	1.95	0.48
1:F:324:THR:HG22	1:F:356:ASP:OD2	2.13	0.48
1:D:210:LEU:O	1:D:213:PRO:HG3	2.12	0.48
1:A:205:THR:HG22	1:A:422:PHE:HA	1.95	0.48
1:F:356:ASP:O	1:F:358:ASP:N	2.46	0.48
1:C:260:GLY:O	1:C:316:VAL:HA	2.13	0.48
1:C:364:ARG:HH21	1:C:447:ARG:HD2	1.79	0.48
1:B:187:ILE:HD12	2:B:602:MYA:H7MA	1.94	0.48
1:D:177:LEU:HD22	1:F:19:LEU:HD12	1.95	0.48
1:A:14:LEU:HD21	1:A:213:PRO:HG3	1.95	0.48
1:A:75:LEU:H	1:A:75:LEU:HD23	1.78	0.48
1:B:165:SER:HB3	1:B:201:HIS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:252:LEU:HD21	1:F:385:CYS:HB3	1.95	0.48
1:B:297:ASN:ND2	1:B:351:TYR:HE2	2.11	0.48
1:B:229:LEU:HD11	1:B:395:VAL:HB	1.96	0.48
1:F:237:LEU:HD21	1:F:241:HIS:O	2.14	0.48
1:E:151:ALA:HB1	1:E:166:VAL:HG22	1.95	0.48
1:E:214:VAL:HG21	1:E:424:LEU:HG	1.96	0.48
1:E:183:THR:HB	1:E:184:PRO:HD3	1.95	0.48
1:E:68:ILE:HG13	1:E:195:ASN:HB3	1.96	0.48
1:A:115:TYR:CE2	1:A:332:LEU:HD11	2.49	0.48
1:F:16:LEU:O	1:F:19:LEU:HD22	2.14	0.48
1:A:243:GLU:O	1:A:247:ILE:HG12	2.14	0.48
1:A:382:TYR:O	1:A:386:ILE:HD12	2.14	0.48
1:C:142:THR:O	1:C:143:GLN:HB2	2.14	0.47
1:A:232:VAL:HG12	1:A:232:VAL:O	2.14	0.47
1:E:242:THR:HG23	1:E:245:ASP:H	1.79	0.47
1:C:401:SER:O	1:C:404:ASN:HB2	2.14	0.47
1:D:124:LEU:HB3	1:D:134:HIS:NE2	2.30	0.47
1:B:38:HIS:HA	2:B:602:MYA:P3X	2.54	0.47
1:D:278:ARG:HD2	1:D:359:PHE:CE1	2.50	0.47
1:E:444:ILE:H	1:E:444:ILE:HD13	1.79	0.47
1:E:130:LYS:HD2	1:E:130:LYS:HA	1.79	0.47
1:B:187:ILE:O	1:B:190:ILE:HG22	2.14	0.47
1:F:232:VAL:HG12	1:F:232:VAL:O	2.14	0.47
1:B:324:THR:HG23	1:B:356:ASP:OD1	2.15	0.47
1:A:93:GLU:O	1:A:97:VAL:HG23	2.15	0.47
1:F:291:LYS:HD2	1:F:292:GLU:N	2.29	0.47
1:E:99:LEU:O	1:E:103:TYR:HB2	2.15	0.47
1:A:272:VAL:HG22	1:A:323:ILE:HG21	1.97	0.47
1:D:404:ASN:HA	1:D:407:PHE:CE2	2.49	0.47
1:E:212:ALA:N	1:E:213:PRO:CD	2.69	0.47
1:F:286:ILE:HD11	1:F:288:ILE:HD13	1.97	0.47
1:A:278:ARG:HD2	1:A:359:PHE:CE1	2.50	0.47
1:A:68:ILE:HG12	1:A:195:ASN:HB3	1.97	0.47
1:E:171:LEU:HB3	2:E:605:MYA:H3A	1.97	0.46
1:A:16:LEU:HD21	1:B:79:PHE:CZ	2.50	0.46
1:B:388:ALA:O	1:B:393:MET:HG3	2.15	0.46
1:B:256:THR:HG22	1:B:383:ASP:CG	2.35	0.46
1:F:148:PHE:O	1:F:171:LEU:HA	2.16	0.46
1:F:88:ASN:HB3	1:F:91:GLN:HB2	1.98	0.46
1:B:353:TYR:OH	1:B:404:ASN:ND2	2.49	0.46
1:F:404:ASN:HD22	1:F:404:ASN:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:ASN:O	1:E:125:LYS:HB2	2.14	0.46
1:E:439:ASP:O	1:E:440:ASN:HB2	2.16	0.46
1:E:256:THR:HG21	1:E:261:LEU:CD1	2.44	0.46
1:D:211:PRO:O	1:D:212:ALA:HB2	2.15	0.46
1:B:222:ARG:NH2	1:B:412:LYS:HG3	2.29	0.46
1:F:190:ILE:O	1:F:194:VAL:HG23	2.15	0.46
1:C:264:LEU:HD11	1:C:272:VAL:HG21	1.97	0.46
1:B:171:LEU:HB2	2:B:602:MYA:C3M	2.45	0.46
1:B:69:SER:OG	1:B:71:LYS:HG2	2.16	0.46
1:F:20:ASN:CG	1:F:21:ASN:H	2.20	0.45
1:F:99:LEU:O	1:F:103:TYR:HB2	2.16	0.45
1:C:238:PRO:O	1:C:241:HIS:HB2	2.16	0.45
1:C:280:GLN:HG2	1:C:283:PHE:HD1	1.79	0.45
1:B:38:HIS:HB3	1:B:41:TRP:HB2	1.98	0.45
1:D:96:PHE:CE2	1:D:117:LYS:HB3	2.51	0.45
1:E:171:LEU:HB2	2:E:605:MYA:H3MA	1.97	0.45
1:B:45:PRO:HB2	1:B:426:ASN:HD22	1.81	0.45
1:E:264:LEU:HD12	1:E:315:VAL:HB	1.99	0.45
1:E:187:ILE:CD1	2:E:605:MYA:H7MA	2.46	0.45
1:E:99:LEU:HD13	1:E:103:TYR:CD1	2.52	0.45
1:A:290:THR:O	1:A:292:GLU:N	2.49	0.45
1:C:218:ARG:HB3	1:C:436:LEU:HD21	1.97	0.45
1:C:113:PHE:HE2	3:C:703:3LP:HAM2	1.81	0.45
1:A:88:ASN:HB3	1:A:91:GLN:HB2	1.98	0.45
1:A:20:ASN:HD22	1:A:417:ASP:HB2	1.82	0.45
1:C:135:ILE:HD11	1:C:193:ARG:HD2	1.98	0.45
1:B:154:VAL:HG21	1:B:167:GLU:HG3	1.98	0.45
1:C:178:ARG:C	1:C:180:LYS:H	2.20	0.45
1:F:59:ILE:HG23	1:F:428:ARG:NH2	2.32	0.45
1:B:171:LEU:HB2	2:B:602:MYA:H3M	1.99	0.44
1:E:99:LEU:HD13	1:E:103:TYR:CE1	2.52	0.44
1:F:333:PRO:HA	1:F:347:ILE:HG12	1.99	0.44
1:D:124:LEU:HB3	1:D:134:HIS:HE2	1.81	0.44
1:D:166:VAL:HG11	1:D:194:VAL:HG11	2.00	0.44
1:B:325:ASP:OD2	1:B:325:ASP:N	2.50	0.44
1:E:114:ASN:HB3	1:E:333:PRO:HG2	1.99	0.44
1:D:312:PHE:HB3	1:D:314:TYR:HE1	1.82	0.44
1:D:388:ALA:O	1:D:393:MET:HG3	2.18	0.44
1:E:60:ASP:N	1:E:426:ASN:HD21	2.14	0.44
1:A:153:PRO:HA	1:A:166:VAL:HA	2.00	0.44
1:F:371:LYS:O	1:F:375:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:LYS:HE2	1:E:345:LEU:HD12	1.99	0.44
1:D:64:THR:C	1:D:66:GLU:H	2.21	0.44
1:A:232:VAL:HG11	1:A:336:ILE:HD13	1.99	0.44
1:A:190:ILE:HD12	1:A:194:VAL:HG23	2.00	0.44
1:E:171:LEU:HD11	1:E:183:THR:HG23	2.00	0.44
1:A:20:ASN:ND2	1:A:417:ASP:O	2.50	0.44
1:E:88:ASN:HB3	1:E:91:GLN:HB2	2.00	0.44
1:E:92:LEU:HD11	1:E:120:PHE:HB3	2.00	0.44
1:C:212:ALA:N	1:C:213:PRO:HD3	2.33	0.44
1:D:232:VAL:O	1:D:232:VAL:CG1	2.65	0.44
1:D:124:LEU:HB3	1:D:134:HIS:CD2	2.53	0.44
1:E:153:PRO:HA	1:E:166:VAL:HG23	1.99	0.43
1:C:85:ASP:H	1:C:91:GLN:NE2	2.15	0.43
1:B:443:ASP:OD2	1:B:446:ARG:HB2	2.18	0.43
1:F:418:GLY:HA3	3:F:706:3LP:CAG	2.49	0.43
1:D:46:VAL:HB	1:D:211:PRO:O	2.18	0.43
1:B:135:ILE:O	1:B:148:PHE:CD1	2.71	0.43
1:B:406:LEU:HG	1:B:447:ARG:HD3	1.99	0.43
1:C:350:LEU:HB2	1:C:396:PHE:CE2	2.53	0.43
1:B:135:ILE:CG2	1:B:136:GLY:N	2.81	0.43
1:A:38:HIS:HB2	1:A:42:ARG:NE	2.33	0.43
1:C:252:LEU:HG	1:C:386:ILE:HG13	2.01	0.43
1:A:262:ARG:HG2	1:A:263:LYS:O	2.19	0.43
1:C:107:ARG:O	1:C:112:ARG:NH2	2.50	0.43
1:F:204:TYR:CD2	2:F:606:MYA:H6MA	2.53	0.43
1:E:187:ILE:HG23	2:E:605:MYA:H9MA	2.00	0.43
1:B:47:LYS:HB3	1:B:212:ALA:CB	2.47	0.43
1:C:341:LYS:HD2	1:C:342:TYR:CZ	2.54	0.43
1:D:336:ILE:HD11	1:D:345:LEU:HB2	2.01	0.43
1:C:106:ASP:HB3	1:C:109:ALA:HB2	2.01	0.43
1:B:168:ILE:HG21	2:B:602:MYA:H7M	2.00	0.43
1:A:49:PHE:CZ	1:A:211:PRO:HA	2.54	0.43
1:C:336:ILE:CD1	1:C:345:LEU:HB2	2.44	0.43
1:E:19:LEU:HG	1:F:176:GLN:HG2	2.01	0.43
1:D:99:LEU:HD12	1:D:120:PHE:CZ	2.51	0.43
1:D:332:LEU:HB3	1:D:349:TYR:CE1	2.54	0.43
1:F:205:THR:HB	1:F:420:LEU:CD2	2.49	0.43
1:C:69:SER:HB3	1:C:71:LYS:HG2	2.01	0.43
1:D:212:ALA:N	1:D:213:PRO:CD	2.63	0.43
1:C:211:PRO:O	1:C:212:ALA:HB3	2.19	0.43
1:E:98:LEU:HD13	1:E:145:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:THR:O	1:D:143:GLN:HB2	2.18	0.42
1:B:202:ALA:HB2	2:B:602:MYA:HCM	2.00	0.42
1:F:378:CYS:O	1:F:382:TYR:HB2	2.18	0.42
1:F:174:HIS:CD2	1:F:176:GLN:HB3	2.52	0.42
1:F:229:LEU:HD23	1:F:345:LEU:HD11	2.00	0.42
1:C:115:TYR:HB3	1:C:120:PHE:CE1	2.55	0.42
1:E:174:HIS:HB3	1:E:177:LEU:HD21	2.00	0.42
1:A:93:GLU:HA	1:A:96:PHE:CE2	2.54	0.42
1:C:137:VAL:HB	1:C:147:ALA:HB3	2.02	0.42
1:F:301:GLU:HB3	1:F:304:LEU:HD11	2.02	0.42
1:D:267:GLU:CD	1:D:267:GLU:H	2.22	0.42
1:B:210:LEU:O	1:B:423:TYR:HE2	2.02	0.42
1:D:53:VAL:HG22	1:D:428:ARG:HG2	2.00	0.42
1:E:382:TYR:HB2	1:E:411:LEU:HD22	2.02	0.42
1:A:174:HIS:CD2	1:A:176:GLN:H	2.36	0.42
1:B:175:LYS:HA	1:B:178:ARG:HD2	2.01	0.42
1:C:363:ASP:HB3	1:C:366:ASP:HB2	2.02	0.42
1:A:206:ALA:HB1	1:A:208:ILE:HD13	2.00	0.42
1:A:224:LEU:HD11	1:A:396:PHE:HB2	2.00	0.42
1:D:93:GLU:HA	1:D:96:PHE:CZ	2.54	0.42
1:A:75:LEU:N	1:A:75:LEU:HD23	2.35	0.42
1:C:357:ALA:HB2	1:C:376:ARG:HG2	2.01	0.42
1:E:127:PRO:HD3	1:E:296:HIS:CD2	2.54	0.42
1:C:174:HIS:CD2	1:C:176:GLN:H	2.38	0.42
1:B:133:TRP:HB3	1:B:151:ALA:HB3	2.02	0.42
1:E:103:TYR:HA	2:E:605:MYA:H7A	2.01	0.42
1:C:16:LEU:HA	1:C:19:LEU:HD22	2.02	0.42
1:A:115:TYR:HB3	1:A:120:PHE:CE1	2.55	0.42
1:D:86:VAL:HG13	1:D:92:LEU:HD13	2.02	0.42
1:D:135:ILE:HD11	1:D:193:ARG:HD2	2.00	0.42
1:F:293:GLU:O	1:F:297:ASN:HB2	2.20	0.42
1:E:202:ALA:HB2	2:E:605:MYA:HEM	2.02	0.42
1:D:151:ALA:CB	1:D:190:ILE:HD11	2.48	0.42
1:B:232:VAL:O	1:B:232:VAL:HG12	2.19	0.42
1:B:99:LEU:HD12	1:B:120:PHE:HZ	1.84	0.42
1:B:156:LEU:HD11	1:B:203:LEU:HB2	2.00	0.42
1:D:112:ARG:HB2	1:D:335:THR:HB	2.01	0.42
1:F:418:GLY:N	3:F:706:3LP:HAG1	2.35	0.42
1:D:168:ILE:HG21	2:D:604:MYA:H8M	2.00	0.42
1:D:405:THR:HG21	1:D:444:ILE:HA	2.01	0.42
1:C:277:LYS:HZ3	1:C:288:ILE:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:ALA:O	1:E:393:MET:HG3	2.20	0.42
1:B:73:LEU:HD13	1:B:188:LYS:HB3	2.01	0.42
1:C:127:PRO:HD3	1:C:296:HIS:CD2	2.55	0.42
1:B:151:ALA:CB	1:B:190:ILE:HD11	2.45	0.41
1:E:290:THR:C	1:E:292:GLU:H	2.24	0.41
1:A:205:THR:HB	1:A:420:LEU:HD22	2.02	0.41
1:F:315:VAL:HG23	1:F:326:PHE:HB2	2.02	0.41
1:B:373:LEU:HD22	1:B:377:LEU:HG	2.02	0.41
1:C:405:THR:CG2	1:C:444:ILE:HA	2.50	0.41
1:D:279:TYR:O	1:D:282:ARG:HG2	2.20	0.41
1:B:187:ILE:CG2	2:B:602:MYA:H9M	2.50	0.41
1:C:406:LEU:HG	1:C:447:ARG:HD3	2.01	0.41
1:A:347:ILE:HG22	1:A:349:TYR:CE1	2.55	0.41
1:E:324:THR:HB	1:E:325:ASP:OD2	2.21	0.41
1:F:402:GLN:HB2	1:F:404:ASN:ND2	2.36	0.41
1:F:272:VAL:HG22	1:F:323:ILE:HG21	2.03	0.41
1:C:275:LEU:HD21	1:C:325:ASP:HA	2.03	0.41
1:D:346:GLY:HA3	1:D:393:MET:HA	2.03	0.41
1:F:420:LEU:HD23	1:F:420:LEU:HA	1.96	0.41
1:F:455:LEU:O	3:F:706:3LP:HAI2	2.20	0.41
1:E:224:LEU:HD21	1:E:396:PHE:HB2	2.01	0.41
1:A:190:ILE:HD13	1:A:190:ILE:HA	1.94	0.41
1:E:93:GLU:HA	1:E:96:PHE:CE2	2.55	0.41
1:A:190:ILE:HG23	2:A:601:MYA:HCMA	2.02	0.41
1:A:211:PRO:O	1:A:212:ALA:CB	2.68	0.41
1:C:135:ILE:HD13	1:C:190:ILE:HD12	2.01	0.41
1:F:53:VAL:HG11	1:F:428:ARG:HB3	2.02	0.41
1:C:174:HIS:HB3	1:C:177:LEU:CD2	2.51	0.41
1:E:211:PRO:O	1:E:212:ALA:CB	2.68	0.41
1:B:238:PRO:O	1:B:241:HIS:HB2	2.20	0.41
1:F:158:VAL:O	1:F:160:GLY:N	2.53	0.41
1:F:224:LEU:HD21	1:F:396:PHE:HB2	2.03	0.41
1:E:404:ASN:O	1:E:408:LEU:HG	2.21	0.41
1:F:93:GLU:HA	1:F:96:PHE:CZ	2.56	0.41
1:D:383:ASP:O	1:D:387:LEU:HG	2.21	0.41
2:C:603:MYA:H3	2:C:603:MYA:HN6A	1.86	0.41
1:E:151:ALA:HB2	1:E:168:ILE:HG13	2.03	0.41
1:F:174:HIS:HB3	1:F:177:LEU:CD2	2.50	0.41
1:C:280:GLN:C	1:C:282:ARG:H	2.24	0.41
1:F:341:LYS:HE3	1:F:341:LYS:HB2	1.89	0.41
1:F:64:THR:HB	1:F:65:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:LEU:HA	1:E:253:PRO:HD3	1.93	0.41
1:E:290:THR:O	1:E:292:GLU:N	2.54	0.41
1:E:232:VAL:O	1:E:232:VAL:CG1	2.69	0.41
1:E:286:ILE:HG22	1:E:451:GLY:HA3	2.03	0.41
1:C:85:ASP:HB3	1:C:91:GLN:HE22	1.87	0.40
1:B:205:THR:HB	1:B:420:LEU:CD2	2.51	0.40
1:F:205:THR:HA	1:F:421:ASN:O	2.21	0.40
1:A:40:PHE:HE1	1:A:188:LYS:HG3	1.86	0.40
1:D:136:GLY:HA2	1:D:148:PHE:HA	2.03	0.40
1:D:397:ASN:HD22	1:D:397:ASN:N	2.19	0.40
1:A:73:LEU:HD23	1:A:74:PRO:HD2	2.03	0.40
1:B:293:GLU:O	1:B:297:ASN:HB2	2.21	0.40
1:E:336:ILE:HD11	1:E:345:LEU:HB2	2.04	0.40
1:E:137:VAL:HB	1:E:147:ALA:HB3	2.03	0.40
1:F:282:ARG:HD3	1:F:364:ARG:HD2	2.04	0.40
1:F:40:PHE:HE1	1:F:188:LYS:HE3	1.86	0.40
1:C:229:LEU:HD11	1:C:395:VAL:HB	2.04	0.40
1:E:242:THR:HG22	1:E:245:ASP:CG	2.42	0.40
1:D:133:TRP:CE2	1:D:194:VAL:HG22	2.57	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	431/455 (95%)	381 (88%)	45 (10%)	5 (1%)	16 56
1	B	431/455 (95%)	399 (93%)	23 (5%)	9 (2%)	9 40
1	C	431/455 (95%)	378 (88%)	47 (11%)	6 (1%)	14 51
1	D	431/455 (95%)	384 (89%)	41 (10%)	6 (1%)	14 51
1	E	431/455 (95%)	380 (88%)	44 (10%)	7 (2%)	12 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	431/455 (95%)	387 (90%)	39 (9%)	5 (1%)	16	56
All	All	2586/2730 (95%)	2309 (89%)	239 (9%)	38 (2%)	13	50

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ALA
1	D	212	ALA
1	E	78	SER
1	E	212	ALA
1	F	69	SER
1	F	212	ALA
1	F	357	ALA
1	A	39	LYS
1	A	78	SER
1	A	291	LYS
1	B	78	SER
1	B	159	ARG
1	B	160	GLY
1	B	211	PRO
1	C	89	LYS
1	C	212	ALA
1	D	78	SER
1	E	76	LEU
1	B	413	PHE
1	C	197	CYS
1	C	269	ILE
1	D	303	SER
1	E	291	LYS
1	F	78	SER
1	F	159	ARG
1	B	291	LYS
1	D	20	ASN
1	D	65	PRO
1	C	179	SER
1	D	438	PRO
1	B	269	ILE
1	B	362	LYS
1	C	431	PRO
1	E	320	ASP
1	B	212	ALA
1	E	269	ILE

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Mol	Chain	Res	Type
1	E	321	GLY
1	A	431	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/413 (95%)	362 (92%)	31 (8%)	15	48
1	B	393/413 (95%)	359 (91%)	34 (9%)	13	43
1	C	393/413 (95%)	363 (92%)	30 (8%)	16	51
1	D	393/413 (95%)	357 (91%)	36 (9%)	11	40
1	E	393/413 (95%)	356 (91%)	37 (9%)	11	39
1	F	393/413 (95%)	361 (92%)	32 (8%)	15	47
All	All	2358/2478 (95%)	2158 (92%)	200 (8%)	13	45

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	52	LYS
1	A	60	ASP
1	A	73	LEU
1	A	75	LEU
1	A	76	LEU
1	A	103	TYR
1	A	130	LYS
1	A	132	ASP
1	A	149	ILE
1	A	171	LEU
1	A	172	CYS
1	A	177	LEU
1	A	190	ILE
1	A	195	ASN
1	A	198	ASP

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Mol	Chain	Res	Type
1	A	208	ILE
1	A	222	ARG
1	A	252	LEU
1	A	261	LEU
1	A	278	ARG
1	A	286	ILE
1	A	291	LYS
1	A	292	GLU
1	A	302	GLU
1	A	311	ILE
1	A	332	LEU
1	A	335	THR
1	A	340	THR
1	A	373	LEU
1	A	420	LEU
1	B	19	LEU
1	B	46	VAL
1	B	66	GLU
1	B	73	LEU
1	B	75	LEU
1	B	114	ASN
1	B	130	LYS
1	B	150	SER
1	B	165	SER
1	B	166	VAL
1	B	171	LEU
1	B	190	ILE
1	B	200	TRP
1	B	242	THR
1	B	247	ILE
1	B	252	LEU
1	B	256	THR
1	B	261	LEU
1	B	267	GLU
1	B	278	ARG
1	B	291	LYS
1	B	297	ASN
1	B	311	ILE
1	B	320	ASP
1	B	325	ASP
1	B	326	PHE
1	B	332	LEU

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Mol	Chain	Res	Type
1	B	336	ILE
1	B	340	THR
1	B	344	ASP
1	B	373	LEU
1	B	381	ILE
1	B	420	LEU
1	B	428	ARG
1	C	19	LEU
1	C	99	LEU
1	C	103	TYR
1	C	108	ASP
1	C	130	LYS
1	C	132	ASP
1	C	152	ILE
1	C	158	VAL
1	C	168	ILE
1	C	171	LEU
1	C	176	GLN
1	C	177	LEU
1	C	200	TRP
1	C	221	HIS
1	C	232	VAL
1	C	242	THR
1	C	261	LEU
1	C	280	GLN
1	C	290	THR
1	C	291	LYS
1	C	320	ASP
1	C	325	ASP
1	C	326	PHE
1	C	335	THR
1	C	340	THR
1	C	351	TYR
1	C	373	LEU
1	C	375	THR
1	C	420	LEU
1	C	444	ILE
1	D	10	LEU
1	D	21	ASN
1	D	68	ILE
1	D	75	LEU
1	D	96	PHE

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Mol	Chain	Res	Type
1	D	103	TYR
1	D	112	ARG
1	D	116	THR
1	D	134	HIS
1	D	149	ILE
1	D	161	LYS
1	D	165	SER
1	D	177	LEU
1	D	190	ILE
1	D	196	LYS
1	D	197	CYS
1	D	208	ILE
1	D	222	ARG
1	D	261	LEU
1	D	268	ASP
1	D	278	ARG
1	D	286	ILE
1	D	288	ILE
1	D	291	LYS
1	D	311	ILE
1	D	325	ASP
1	D	326	PHE
1	D	332	LEU
1	D	373	LEU
1	D	397	ASN
1	D	399	LEU
1	D	405	THR
1	D	410	ASP
1	D	420	LEU
1	D	432	ILE
1	D	452	VAL
1	E	18	GLN
1	E	19	LEU
1	E	60	ASP
1	E	66	GLU
1	E	99	LEU
1	E	103	TYR
1	E	105	GLU
1	E	121	ASN
1	E	130	LYS
1	E	132	ASP
1	E	152	ILE

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Mol	Chain	Res	Type
1	E	168	ILE
1	E	171	LEU
1	E	176	GLN
1	E	208	ILE
1	E	210	LEU
1	E	229	LEU
1	E	249	GLU
1	E	256	THR
1	E	261	LEU
1	E	268	ASP
1	E	291	LYS
1	E	311	ILE
1	E	324	THR
1	E	325	ASP
1	E	326	PHE
1	E	332	LEU
1	E	335	THR
1	E	344	ASP
1	E	351	TYR
1	E	373	LEU
1	E	397	ASN
1	E	405	THR
1	E	410	ASP
1	E	420	LEU
1	E	442	ASN
1	E	444	ILE
1	F	19	LEU
1	F	60	ASP
1	F	75	LEU
1	F	82	CYS
1	F	99	LEU
1	F	105	GLU
1	F	130	LYS
1	F	152	ILE
1	F	171	LEU
1	F	176	GLN
1	F	177	LEU
1	F	200	TRP
1	F	222	ARG
1	F	239	ASP
1	F	278	ARG
1	F	285	LEU

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Mol	Chain	Res	Type
1	F	291	LYS
1	F	292	GLU
1	F	311	ILE
1	F	315	VAL
1	F	324	THR
1	F	325	ASP
1	F	326	PHE
1	F	340	THR
1	F	347	ILE
1	F	351	TYR
1	F	373	LEU
1	F	375	THR
1	F	392	ASN
1	F	420	LEU
1	F	426	ASN
1	F	452	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	114	ASN
1	A	174	HIS
1	A	176	GLN
1	A	195	ASN
1	A	296	HIS
1	A	297	ASN
1	A	318	GLN
1	A	397	ASN
1	A	404	ASN
1	A	426	ASN
1	B	114	ASN
1	B	174	HIS
1	B	195	ASN
1	B	241	HIS
1	B	297	ASN
1	B	397	ASN
1	B	404	ASN
1	B	426	ASN
1	C	18	GLN
1	C	91	GLN
1	C	114	ASN

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Mol	Chain	Res	Type
1	C	195	ASN
1	C	397	ASN
1	C	421	ASN
1	C	426	ASN
1	D	18	GLN
1	D	176	GLN
1	D	195	ASN
1	D	390	ASN
1	D	397	ASN
1	D	421	ASN
1	D	426	ASN
1	E	18	GLN
1	E	176	GLN
1	E	195	ASN
1	E	397	ASN
1	E	421	ASN
1	E	426	ASN
1	F	20	ASN
1	F	91	GLN
1	F	174	HIS
1	F	402	GLN
1	F	404	ASN
1	F	421	ASN
1	F	426	ASN
1	F	437	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MYA	A	601	-	53,65,65	0.75	2 (3%)	65,91,91	1.92	7 (10%)
2	MYA	B	602	-	53,65,65	0.71	1 (1%)	65,91,91	1.84	10 (15%)
2	MYA	C	603	-	53,65,65	0.71	1 (1%)	65,91,91	1.86	10 (15%)
3	3LP	C	703	-	25,28,28	0.78	0	25,39,39	1.25	5 (20%)
2	MYA	D	604	-	53,65,65	0.73	1 (1%)	65,91,91	1.93	9 (13%)
2	MYA	E	605	-	53,65,65	0.71	1 (1%)	65,91,91	1.84	7 (10%)
2	MYA	F	606	-	53,65,65	0.73	2 (3%)	65,91,91	1.93	8 (12%)
3	3LP	F	706	-	25,28,28	0.81	1 (4%)	25,39,39	1.38	6 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYA	A	601	-	1/1/12/14	0/59/80/80	0/3/3/3
2	MYA	B	602	-	1/1/12/14	0/59/80/80	0/3/3/3
2	MYA	C	603	-	1/1/12/14	0/59/80/80	0/3/3/3
3	3LP	C	703	-	-	0/7/24/24	0/4/4/4
2	MYA	D	604	-	1/1/12/14	0/59/80/80	0/3/3/3
2	MYA	E	605	-	1/1/12/14	0/59/80/80	0/3/3/3
2	MYA	F	606	-	1/1/12/14	0/59/80/80	0/3/3/3
3	3LP	F	706	-	-	0/7/24/24	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	MYA	C2-S1	-3.57	1.76	1.81
2	E	605	MYA	C2-S1	-3.45	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	604	MYA	C2-S1	-3.43	1.76	1.81
2	F	606	MYA	C2-S1	-3.23	1.77	1.81
2	C	603	MYA	C2-S1	-3.20	1.77	1.81
2	B	602	MYA	C2-S1	-3.17	1.77	1.81
3	F	706	3LP	CAS-CAU	-2.15	1.37	1.41
2	F	606	MYA	O4X-C1X	2.04	1.43	1.41
2	A	601	MYA	O4X-C1X	2.20	1.44	1.41

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	606	MYA	N3A-C2A-N1A	-10.45	120.89	128.89
2	A	601	MYA	N3A-C2A-N1A	-10.40	120.93	128.89
2	E	605	MYA	N3A-C2A-N1A	-10.30	121.00	128.89
2	C	603	MYA	N3A-C2A-N1A	-10.28	121.02	128.89
2	B	602	MYA	N3A-C2A-N1A	-10.03	121.22	128.89
2	D	604	MYA	N3A-C2A-N1A	-9.83	121.36	128.89
2	D	604	MYA	C2-C3-N4	-4.34	103.67	112.36
3	F	706	3LP	CAH-CAL-CAT	-3.46	107.26	113.18
2	E	605	MYA	P2A-O3A-P1A	-3.42	123.13	132.73
2	A	601	MYA	C2-C3-N4	-3.41	105.53	112.36
2	D	604	MYA	P2A-O3A-P1A	-3.27	123.55	132.73
2	F	606	MYA	P2A-O3A-P1A	-3.22	123.67	132.73
2	E	605	MYA	C2-C3-N4	-3.03	106.29	112.36
2	C	603	MYA	P2A-O3A-P1A	-3.00	124.30	132.73
2	B	602	MYA	C6-C7-N8	-2.93	105.45	111.88
2	B	602	MYA	P2A-O3A-P1A	-2.90	124.60	132.73
2	F	606	MYA	C2-C3-N4	-2.85	106.66	112.36
3	C	703	3LP	CAH-CAL-CAT	-2.78	108.41	113.18
2	A	601	MYA	P2A-O3A-P1A	-2.72	125.10	132.73
2	F	606	MYA	O3X-P3X-O9A	-2.66	100.47	107.11
3	F	706	3LP	CAR-CAE-CAU	-2.49	118.55	121.62
2	D	604	MYA	C4A-C5A-N7A	-2.45	107.22	109.48
2	C	603	MYA	C2-C3-N4	-2.40	107.55	112.36
3	C	703	3LP	CAR-CAE-CAU	-2.32	118.76	121.62
2	E	605	MYA	C4A-C5A-N7A	-2.30	107.36	109.48
3	F	706	3LP	CAG-CAK-CAS	-2.30	108.53	112.22
2	C	603	MYA	C4A-C5A-N7A	-2.25	107.41	109.48
2	B	602	MYA	C4A-C5A-N7A	-2.20	107.45	109.48
2	B	602	MYA	C2-C3-N4	-2.19	107.97	112.36
2	A	601	MYA	C6-C7-N8	-2.17	107.11	111.88
3	C	703	3LP	CAG-CAK-CAS	-2.15	108.76	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	MYA	C13-C11-C12	-2.11	105.76	108.50
2	C	603	MYA	C6-C7-N8	-2.08	107.32	111.88
3	F	706	3LP	CAD-CAV-CAU	-2.05	118.11	120.93
2	D	604	MYA	C2X-C1X-N9A	-2.02	111.21	114.29
2	C	603	MYA	C7-N8-C9	2.03	126.54	122.53
3	C	703	3LP	CAI-CAM-CAX	2.06	114.32	111.13
2	C	603	MYA	C3-N4-C5	2.09	126.90	122.79
3	F	706	3LP	CAI-CAM-CAX	2.11	114.40	111.13
2	B	602	MYA	C14-C11-C10	2.12	113.22	109.34
2	E	605	MYA	C14-C11-C10	2.20	113.35	109.34
3	C	703	3LP	CAE-CAU-CAV	2.24	122.33	119.65
2	F	606	MYA	C3-N4-C5	2.25	127.21	122.79
2	D	604	MYA	C14-C11-C10	2.29	113.52	109.34
2	E	605	MYA	C3-N4-C5	2.29	127.30	122.79
2	A	601	MYA	C3-N4-C5	2.32	127.35	122.79
2	F	606	MYA	C2-S1-C2M	2.37	103.82	100.40
2	F	606	MYA	C7-N8-C9	2.44	127.36	122.53
3	F	706	3LP	CAE-CAU-CAV	2.55	122.70	119.65
2	D	604	MYA	C7-N8-C9	2.59	127.65	122.53
2	B	602	MYA	C2-S1-C2M	2.62	104.18	100.40
2	A	601	MYA	C7-N8-C9	2.68	127.83	122.53
2	B	602	MYA	C7-N8-C9	2.81	128.10	122.53
2	D	604	MYA	C3-N4-C5	2.82	128.34	122.79
2	B	602	MYA	C3-N4-C5	2.91	128.51	122.79
2	C	603	MYA	C2-S1-C2M	3.07	104.84	100.40
2	C	603	MYA	O2M-C2M-C3M	5.10	118.38	109.05
2	E	605	MYA	O2M-C2M-C3M	5.52	119.15	109.05
2	B	602	MYA	O2M-C2M-C3M	5.57	119.24	109.05
2	F	606	MYA	O2M-C2M-C3M	6.22	120.42	109.05
2	A	601	MYA	O2M-C2M-C3M	6.89	121.64	109.05
2	D	604	MYA	O2M-C2M-C3M	6.93	121.73	109.05

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	604	MYA	C10
2	C	603	MYA	C10
2	A	601	MYA	C10
2	F	606	MYA	C10
2	E	605	MYA	C10
2	B	602	MYA	C10

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	MYA	3	0
2	B	602	MYA	11	0
2	C	603	MYA	5	0
3	C	703	3LP	4	0
2	D	604	MYA	3	0
2	E	605	MYA	9	0
2	F	606	MYA	4	0
3	F	706	3LP	10	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	435/455 (95%)	-0.61	0	100	100	11, 30, 58, 80	0
1	B	435/455 (95%)	-0.68	0	100	100	11, 24, 47, 81	0
1	C	435/455 (95%)	-0.40	1 (0%)	95	87	13, 40, 77, 95	0
1	D	435/455 (95%)	-0.58	0	100	100	12, 29, 59, 82	0
1	E	435/455 (95%)	-0.64	0	100	100	11, 26, 54, 79	0
1	F	435/455 (95%)	-0.47	1 (0%)	95	87	11, 36, 77, 93	0
All	All	2610/2730 (95%)	-0.56	2 (0%)	95	90	11, 30, 73, 95	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	ASP	2.5
1	F	52	LYS	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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	3LP	C	703	25/25	0.74	0.38	6.12	71,72,73,74	0
3	3LP	F	706	25/25	0.73	0.35	4.70	71,72,73,74	0
2	MYA	F	606	63/63	0.91	0.20	-0.14	39,40,51,52	0
2	MYA	E	605	63/63	0.95	0.13	-0.35	16,31,36,36	0
2	MYA	B	602	63/63	0.95	0.14	-0.50	23,26,28,28	0
2	MYA	C	603	63/63	0.93	0.16	-0.55	41,43,49,49	0
2	MYA	A	601	63/63	0.95	0.14	-0.60	25,38,44,44	0
2	MYA	D	604	63/63	0.95	0.13	-0.83	18,30,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.