



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:03 AM GMT

PDB ID : 2P6E
Title : Crystal structures of *Saccharomyces cerevisiae* N-myristoyltransferase with bound myristoyl-CoA
Authors : Wu, J.; Ding, J.
Deposited on : 2007-03-18
Resolution : 2.90 Å(reported)

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

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

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

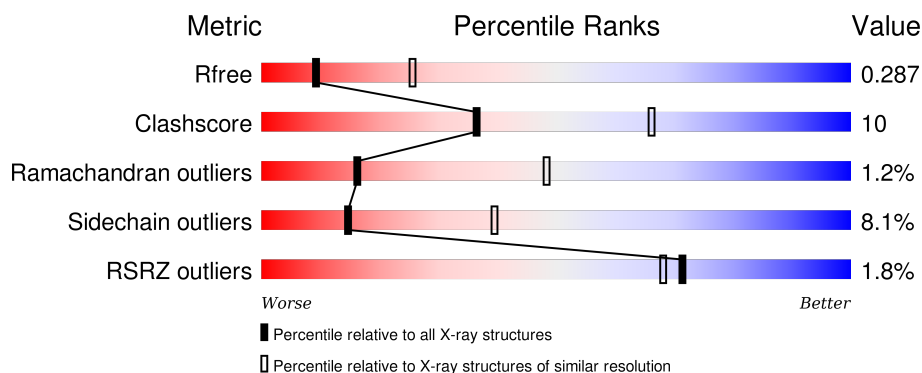
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




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

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

Mol	Chain	Length	Quality of chain
1	A	455	<div> <div>2%</div> <div>73% 21% . .</div> </div>
1	B	455	<div> <div>%</div> <div>70% 23% . .</div> </div>
1	C	455	<div> <div>2%</div> <div>73% 22% . .</div> </div>
1	D	455	<div> <div>2%</div> <div>75% 20% . .</div> </div>
1	E	455	<div> <div>2%</div> <div>69% 27% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	455	

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	-	-	-

2 Entry composition [i](#)

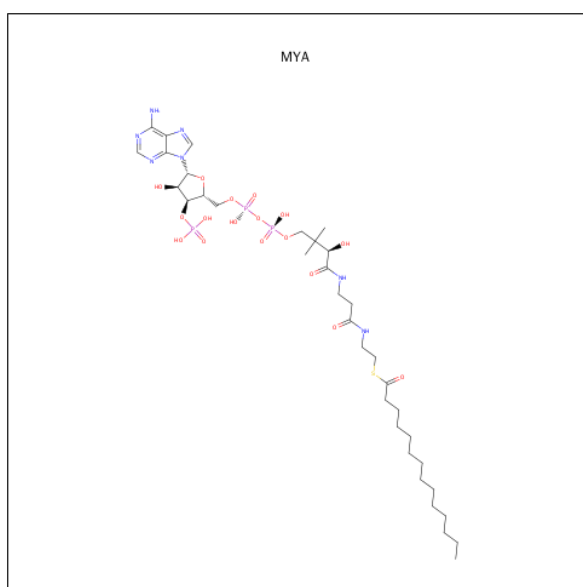
There are 2 unique types of molecules in this entry. The entry contains 22163 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	442	Total	C	N	O	S	0	0	0
			3627	2348	603	667	9			
1	B	443	Total	C	N	O	S	0	0	0
			3634	2352	604	669	9			
1	C	446	Total	C	N	O	S	0	0	0
			3661	2367	608	677	9			
1	D	443	Total	C	N	O	S	0	0	0
			3636	2354	605	668	9			
1	E	443	Total	C	N	O	S	0	0	0
			3634	2352	604	669	9			
1	F	438	Total	C	N	O	S	0	0	0
			3593	2326	598	660	9			

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

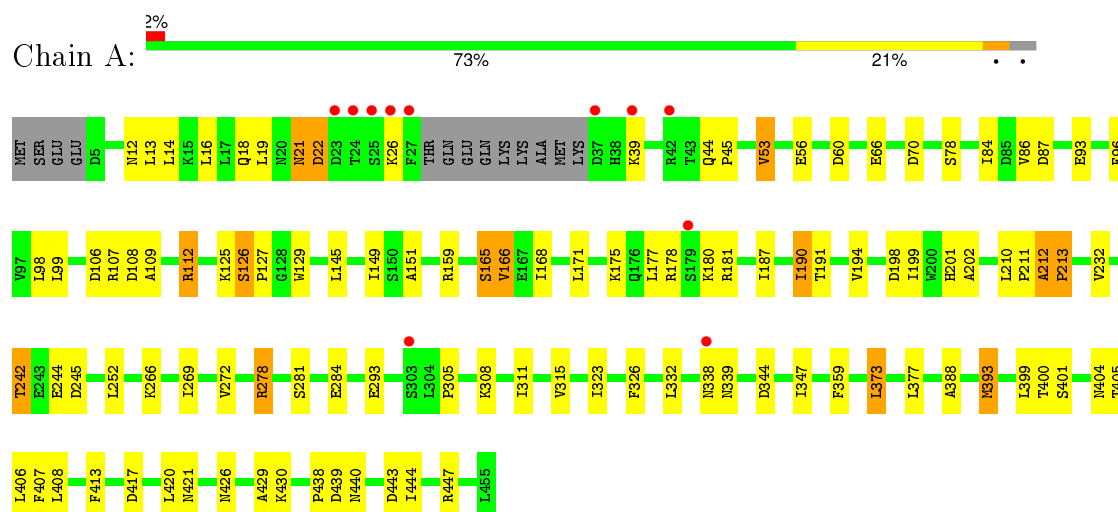


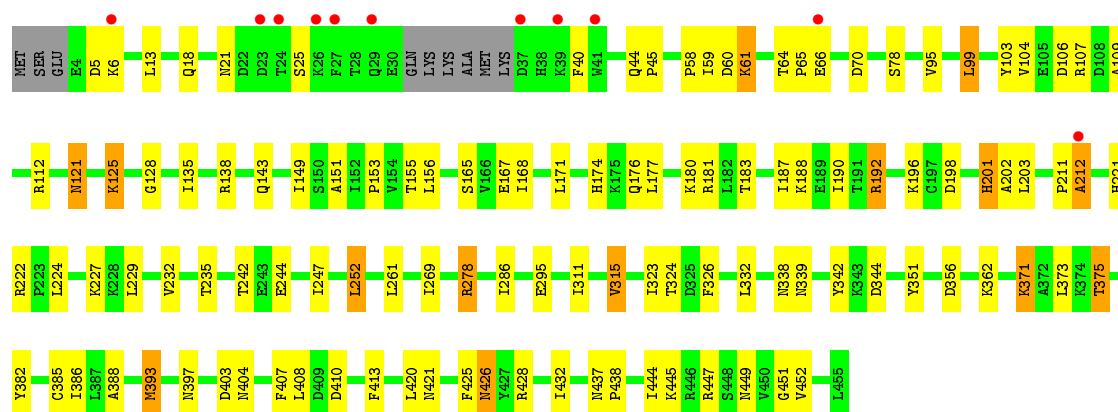
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0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

3 Residue-property plots

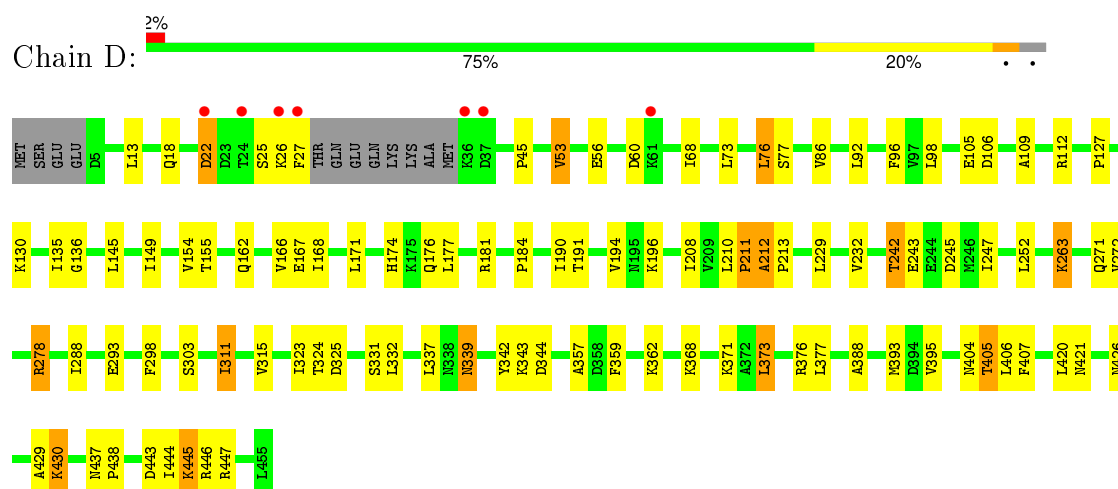
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

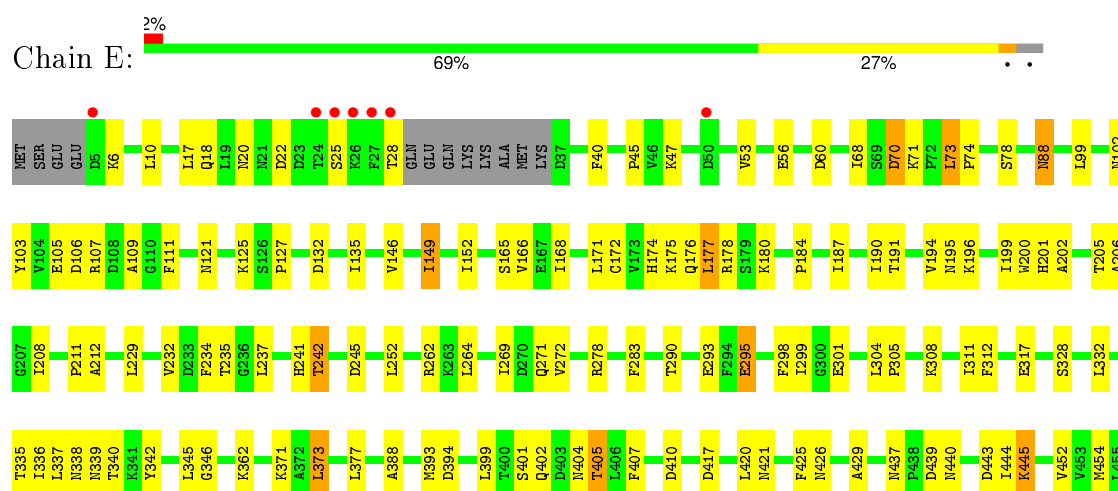




• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

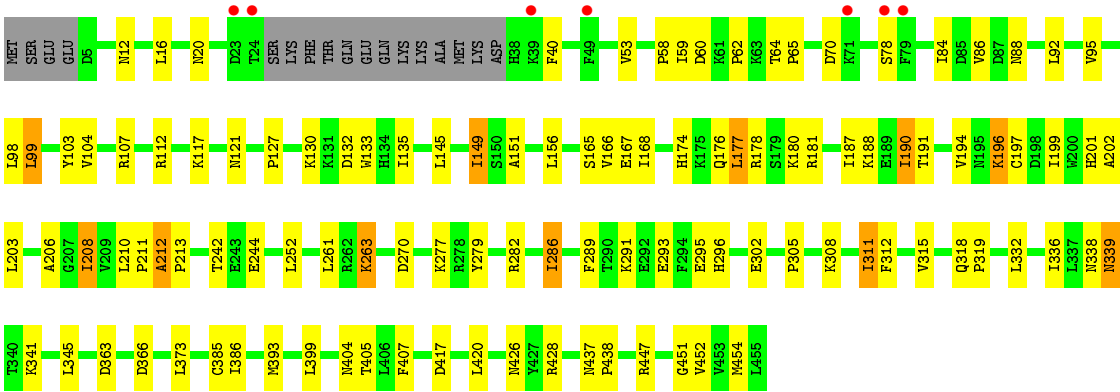


• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.22Å 150.87Å 134.05Å 90.00° 107.65° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 49.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.90) 98.4 (49.38-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.249 , 0.262 0.245 , 0.287	Depositor DCC
R_{free} test set	3947 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	4 of 107688 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22163	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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 51.56 % 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 5.5100e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.36	0/3716	0.53	0/5024
1	B	0.37	0/3723	0.54	0/5034
1	C	0.37	0/3750	0.54	0/5070
1	D	0.37	0/3725	0.55	0/5035
1	E	0.37	0/3723	0.54	0/5034
1	F	0.36	0/3681	0.53	0/4978
All	All	0.37	0/22318	0.54	0/30175

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3627	0	3615	78	0
1	B	3634	0	3622	69	0
1	C	3661	0	3642	70	0
1	D	3636	0	3628	60	0
1	E	3634	0	3622	78	0
1	F	3593	0	3584	61	0
2	A	63	0	58	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	63	0	58	5	0
2	C	63	0	58	6	0
2	D	63	0	58	2	0
2	E	63	0	58	8	0
2	F	63	0	58	5	0
All	All	22163	0	22061	420	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 (420) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ARG:HG3	1:C:278:ARG:HH11	1.07	1.15
1:B:278:ARG:HH11	1:B:278:ARG:HG3	1.00	1.10
1:A:212:ALA:H	1:A:213:PRO:HD3	1.10	1.07
1:A:151:ALA:HB2	1:A:190:ILE:HD11	1.35	1.05
1:B:47:LYS:HD2	1:B:212:ALA:HB1	1.43	1.01
1:D:76:LEU:HD23	1:D:76:LEU:H	1.36	0.91
1:A:212:ALA:H	1:A:213:PRO:CD	1.83	0.90
1:B:278:ARG:HG3	1:B:278:ARG:NH1	1.80	0.89
1:E:70:ASP:HB3	1:E:196:LYS:HE3	1.54	0.89
1:A:190:ILE:O	1:A:194:VAL:HG23	1.73	0.89
1:A:60:ASP:H	1:A:426:ASN:HD21	1.17	0.87
1:A:112:ARG:HH11	1:A:112:ARG:CG	1.87	0.87
1:C:278:ARG:HG3	1:C:278:ARG:NH1	1.86	0.86
1:E:339:ASN:HD22	1:E:342:TYR:H	1.22	0.85
1:C:437:ASN:HB3	1:C:438:PRO:HD2	1.60	0.84
1:D:60:ASP:H	1:D:426:ASN:HD21	1.25	0.84
1:F:336:ILE:HD11	1:F:345:LEU:HB2	1.59	0.83
1:B:60:ASP:H	1:B:426:ASN:HD21	1.29	0.80
1:C:60:ASP:H	1:C:426:ASN:HD21	1.28	0.80
1:E:339:ASN:ND2	1:E:342:TYR:H	1.81	0.79
1:D:278:ARG:HD2	1:D:359:PHE:CE1	2.18	0.78
1:D:211:PRO:O	1:D:212:ALA:CB	2.31	0.78
1:E:47:LYS:HD2	1:E:212:ALA:HB1	1.66	0.77
1:A:212:ALA:N	1:A:213:PRO:HD3	1.95	0.77
1:D:405:THR:HG21	1:D:443:ASP:O	1.84	0.77
1:A:112:ARG:HG2	1:A:112:ARG:HH11	1.48	0.77
1:B:135:ILE:HD13	1:B:190:ILE:HD13	1.69	0.75
1:A:106:ASP:HB3	1:A:109:ALA:HB2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:THR:HG21	1:E:443:ASP:O	1.87	0.75
1:F:263:LYS:H	1:F:263:LYS:HE3	1.50	0.74
1:F:339:ASN:HD22	1:F:341:LYS:H	1.33	0.74
1:B:70:ASP:HB3	1:B:196:LYS:HE3	1.69	0.73
1:D:211:PRO:O	1:D:212:ALA:HB2	1.89	0.73
1:E:388:ALA:O	1:E:393:MET:HG3	1.88	0.73
1:A:194:VAL:HG12	1:A:199:ILE:HB	1.70	0.72
1:A:388:ALA:O	1:A:393:MET:HG3	1.89	0.72
1:B:229:LEU:HB3	1:B:235:THR:HG22	1.71	0.72
1:F:212:ALA:H	1:F:213:PRO:HD3	1.55	0.72
1:F:404:ASN:HA	1:F:407:PHE:CE2	2.25	0.71
1:D:168:ILE:HG13	2:D:604:MYA:HBMA	1.72	0.71
1:C:371:LYS:O	1:C:375:THR:HG22	1.91	0.71
1:B:278:ARG:HH11	1:B:278:ARG:CG	1.93	0.70
1:C:339:ASN:HD22	1:C:342:TYR:H	1.36	0.70
1:D:406:LEU:HG	1:D:447:ARG:HD3	1.72	0.70
1:A:405:THR:CG2	1:A:444:ILE:HA	2.22	0.70
1:E:18:GLN:HE22	1:E:421:ASN:HD21	1.39	0.70
1:D:76:LEU:HD23	1:D:76:LEU:N	2.07	0.69
1:A:151:ALA:CB	1:A:190:ILE:HD11	2.16	0.69
1:E:336:ILE:CD1	1:E:345:LEU:HB2	2.22	0.69
1:E:187:ILE:HG12	2:E:605:MYA:H7MA	1.73	0.69
1:A:278:ARG:HD2	1:A:359:PHE:CE1	2.27	0.69
1:D:127:PRO:HG2	1:D:293:GLU:HA	1.75	0.68
1:B:439:ASP:O	1:B:440:ASN:HB2	1.92	0.68
1:A:112:ARG:NH1	1:A:112:ARG:CG	2.55	0.68
1:E:18:GLN:NE2	1:E:421:ASN:HD21	1.91	0.67
1:E:194:VAL:HG12	1:E:199:ILE:HB	1.75	0.67
1:B:339:ASN:HD22	1:B:341:LYS:H	1.42	0.67
1:A:168:ILE:HG21	2:A:601:MYA:H7M	1.77	0.67
1:B:174:HIS:HD2	1:B:176:GLN:H	1.41	0.66
1:F:202:ALA:HB2	2:F:606:MYA:HDMA	1.77	0.66
1:A:22:ASP:HB3	1:A:26:LYS:HD3	1.78	0.66
1:C:278:ARG:CG	1:C:278:ARG:HH11	1.96	0.66
1:F:20:ASN:HB2	1:F:417:ASP:HB2	1.77	0.66
1:C:242:THR:HG22	1:C:244:GLU:H	1.60	0.66
1:B:174:HIS:CD2	1:B:176:GLN:H	2.14	0.66
1:F:12:ASN:O	1:F:16:LEU:HG	1.95	0.66
1:D:242:THR:HG22	1:D:245:ASP:H	1.60	0.65
1:D:60:ASP:H	1:D:426:ASN:ND2	1.95	0.65
1:E:191:THR:HA	2:E:605:MYA:HDM	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:VAL:HG13	1:D:430:LYS:HD3	1.78	0.65
1:E:68:ILE:HD11	1:E:200:TRP:CH2	2.32	0.64
1:B:388:ALA:O	1:B:393:MET:HG3	1.98	0.64
1:B:339:ASN:ND2	1:B:341:LYS:H	1.96	0.64
1:F:212:ALA:H	1:F:213:PRO:CD	2.10	0.64
1:A:60:ASP:H	1:A:426:ASN:ND2	1.92	0.64
1:D:263:LYS:HD3	1:D:263:LYS:H	1.62	0.64
1:D:388:ALA:O	1:D:393:MET:HG3	1.97	0.64
2:E:605:MYA:H6M	2:E:605:MYA:H2AA	1.79	0.63
1:B:336:ILE:HD11	1:B:345:LEU:HB2	1.80	0.63
1:C:18:GLN:HE22	1:C:421:ASN:HD21	1.46	0.63
1:F:64:THR:HB	1:F:65:PRO:HD2	1.79	0.63
1:C:168:ILE:HD11	2:C:603:MYA:HCM	1.80	0.63
1:E:121:ASN:O	1:E:125:LYS:HB2	1.99	0.63
1:C:59:ILE:HG23	1:C:428:ARG:NH2	2.14	0.63
1:F:405:THR:HG22	1:F:447:ARG:HG2	1.81	0.62
1:D:212:ALA:O	1:D:213:PRO:C	2.37	0.62
1:C:168:ILE:HG21	2:C:603:MYA:H7M	1.82	0.62
1:A:127:PRO:HG2	1:A:293:GLU:HA	1.81	0.62
1:C:151:ALA:HA	1:C:167:GLU:O	2.00	0.62
1:C:174:HIS:HB3	1:C:177:LEU:HD21	1.80	0.62
1:F:242:THR:HG22	1:F:244:GLU:H	1.65	0.62
1:E:336:ILE:HD11	1:E:345:LEU:HB2	1.81	0.62
1:B:21:ASN:HB3	1:C:107:ARG:HH22	1.65	0.61
1:A:210:LEU:O	1:A:213:PRO:HD3	2.00	0.61
1:C:121:ASN:O	1:C:125:LYS:HB2	2.00	0.61
1:B:20:ASN:HD22	1:B:417:ASP:HB2	1.65	0.61
1:D:404:ASN:HD22	1:D:407:PHE:HZ	1.43	0.61
1:D:263:LYS:CD	1:D:263:LYS:H	2.13	0.60
1:E:437:ASN:HD21	1:E:445:LYS:HE3	1.65	0.60
1:B:60:ASP:H	1:B:426:ASN:ND2	1.97	0.60
1:D:339:ASN:HD22	1:D:342:TYR:H	1.50	0.60
1:B:242:THR:HB	1:B:245:ASP:H	1.66	0.60
1:D:18:GLN:HE22	1:D:421:ASN:HD21	1.48	0.60
1:C:404:ASN:HA	1:C:407:PHE:CE2	2.37	0.60
1:B:18:GLN:HE22	1:B:421:ASN:HD21	1.49	0.60
1:F:305:PRO:HG2	1:F:308:LYS:HG3	1.82	0.60
1:A:405:THR:HG21	1:A:443:ASP:O	2.03	0.59
1:D:76:LEU:CD2	1:D:76:LEU:N	2.65	0.59
1:C:40:PHE:HE1	1:C:188:LYS:HE3	1.66	0.59
1:C:174:HIS:HB3	1:C:177:LEU:CD2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:PHE:HA	1:B:311:ILE:HG12	1.85	0.59
1:E:373:LEU:HD22	1:E:377:LEU:HG	1.85	0.59
1:E:405:THR:CG2	1:E:444:ILE:HA	2.33	0.59
1:B:405:THR:HG21	1:B:443:ASP:O	2.02	0.59
1:F:211:PRO:O	1:F:212:ALA:HB2	2.03	0.58
1:F:149:ILE:HD11	1:F:168:ILE:HG23	1.86	0.58
1:F:59:ILE:HG23	1:F:428:ARG:NH2	2.19	0.58
1:F:70:ASP:HB3	1:F:196:LYS:HE3	1.86	0.58
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.67	0.57
1:E:60:ASP:H	1:E:426:ASN:HD21	1.52	0.57
1:F:437:ASN:HB3	1:F:438:PRO:CD	2.33	0.57
1:A:305:PRO:HG2	1:A:308:LYS:HG3	1.85	0.57
1:D:437:ASN:HD21	1:D:445:LYS:HE3	1.69	0.57
1:B:56:GLU:HG2	1:B:429:ALA:HA	1.86	0.57
1:A:405:THR:HG22	1:A:444:ILE:HA	1.87	0.57
1:E:168:ILE:HG13	2:E:605:MYA:HAMA	1.85	0.57
1:E:165:SER:HB3	1:E:201:HIS:HB2	1.87	0.57
1:F:174:HIS:HB3	1:F:177:LEU:CD2	2.35	0.57
1:A:212:ALA:N	1:A:213:PRO:CD	2.58	0.57
1:E:190:ILE:O	1:E:194:VAL:HG23	2.04	0.57
1:E:232:VAL:O	1:E:232:VAL:HG12	2.05	0.57
1:F:279:TYR:O	1:F:282:ARG:HG2	2.05	0.57
1:E:290:THR:OG1	1:E:293:GLU:HG2	2.05	0.56
1:F:178:ARG:O	1:F:180:LYS:HG3	2.05	0.56
1:C:61:LYS:H	1:C:61:LYS:HD3	1.70	0.56
1:E:242:THR:HB	1:E:245:ASP:H	1.71	0.56
1:A:242:THR:HG22	1:A:245:ASP:H	1.70	0.56
1:A:202:ALA:HB2	2:A:601:MYA:HCMA	1.86	0.56
1:C:70:ASP:HB3	1:C:196:LYS:HE3	1.87	0.56
1:D:272:VAL:HG22	1:D:323:ILE:HG21	1.87	0.56
1:F:151:ALA:HA	1:F:167:GLU:O	2.06	0.56
1:A:202:ALA:CB	2:A:601:MYA:HCMA	2.35	0.56
1:F:181:ARG:NH2	2:F:606:MYA:O7A	2.39	0.56
1:B:191:THR:HA	2:B:602:MYA:HDM	1.89	0.55
1:F:211:PRO:O	1:F:212:ALA:CB	2.54	0.55
1:C:437:ASN:HB3	1:C:438:PRO:CD	2.34	0.55
1:C:18:GLN:NE2	1:C:421:ASN:HD21	2.03	0.55
1:B:404:ASN:HA	1:B:407:PHE:CE2	2.41	0.55
1:A:56:GLU:HG2	1:A:429:ALA:HA	1.89	0.55
1:C:437:ASN:CB	1:C:438:PRO:HD2	2.34	0.55
1:C:106:ASP:HB3	1:C:109:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLN:NE2	1:B:421:ASN:HD21	2.05	0.55
1:C:40:PHE:CE1	1:C:188:LYS:HE3	2.42	0.54
1:C:99:LEU:O	1:C:103:TYR:HB2	2.07	0.54
1:C:177:LEU:HB2	1:C:180:LYS:HE2	1.89	0.54
1:E:68:ILE:CD1	1:E:195:ASN:HB3	2.37	0.54
1:D:135:ILE:HG22	1:D:136:GLY:H	1.71	0.54
1:E:298:PHE:HA	1:E:311:ILE:HG12	1.90	0.54
1:C:211:PRO:O	1:C:212:ALA:HB2	2.08	0.54
1:B:339:ASN:HD22	1:B:342:TYR:H	1.54	0.54
1:A:86:VAL:HG11	1:A:125:LYS:HG3	1.89	0.54
1:B:444:ILE:HD13	1:B:444:ILE:H	1.73	0.53
1:D:45:PRO:O	1:D:426:ASN:HA	2.08	0.53
1:E:20:ASN:ND2	1:E:22:ASP:HB2	2.23	0.53
2:E:605:MYA:H6M	2:E:605:MYA:C2A	2.38	0.53
1:F:437:ASN:HB3	1:F:438:PRO:HD2	1.90	0.53
1:E:88:ASN:HD22	1:E:88:ASN:C	2.11	0.53
1:B:174:HIS:HB3	1:B:177:LEU:HD21	1.91	0.53
1:F:104:VAL:HG21	1:F:112:ARG:HA	1.91	0.53
1:E:68:ILE:HD13	1:E:195:ASN:HB3	1.90	0.53
1:A:439:ASP:O	1:A:440:ASN:HB2	2.09	0.53
1:E:301:GLU:HB3	1:E:304:LEU:HG	1.91	0.53
1:C:224:LEU:HD12	1:C:393:MET:HB2	1.91	0.53
1:B:283:PHE:CE2	1:B:402:GLN:HA	2.44	0.53
1:F:339:ASN:ND2	1:F:341:LYS:H	2.04	0.52
1:E:401:SER:O	1:E:404:ASN:HB2	2.08	0.52
1:E:305:PRO:HG2	1:E:308:LYS:HG3	1.91	0.52
1:E:237:LEU:HD21	1:E:241:HIS:O	2.10	0.52
1:F:156:LEU:HD11	1:F:203:LEU:HB2	1.91	0.52
1:E:264:LEU:HD11	1:E:272:VAL:HG21	1.92	0.52
1:E:102:ASN:O	1:E:178:ARG:NH2	2.42	0.52
1:C:168:ILE:CD1	2:C:603:MYA:HCM	2.40	0.52
1:A:18:GLN:HE22	1:A:421:ASN:HD21	1.57	0.52
1:A:112:ARG:HG3	1:A:112:ARG:NH1	2.24	0.52
1:A:175:LYS:HA	1:A:178:ARG:HG3	1.92	0.52
1:E:99:LEU:HD22	1:E:172:CYS:CB	2.40	0.52
1:B:371:LYS:HE3	1:B:371:LYS:HA	1.90	0.52
1:A:107:ARG:HD3	1:A:175:LYS:HD3	1.91	0.52
1:C:315:VAL:HG22	1:C:323:ILE:CG2	2.40	0.52
1:C:183:THR:O	1:C:187:ILE:HG12	2.10	0.52
1:A:211:PRO:O	1:A:212:ALA:HB2	2.09	0.52
1:B:102:ASN:O	1:B:178:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:VAL:O	1:B:232:VAL:HG12	2.11	0.52
1:E:47:LYS:HB3	1:E:212:ALA:CB	2.39	0.51
1:B:156:LEU:HG	1:B:165:SER:OG	2.11	0.51
1:B:205:THR:HB	1:B:420:LEU:HD22	1.93	0.51
1:E:194:VAL:CG1	1:E:199:ILE:HB	2.40	0.51
1:D:174:HIS:CD2	1:D:176:GLN:H	2.29	0.51
1:F:206:ALA:HB1	1:F:208:ILE:HD13	1.93	0.51
1:F:99:LEU:O	1:F:103:TYR:HB2	2.11	0.51
1:C:174:HIS:CD2	1:C:176:GLN:H	2.29	0.51
1:A:14:LEU:HD21	1:A:213:PRO:HG2	1.93	0.50
1:D:405:THR:CG2	1:D:444:ILE:HA	2.40	0.50
1:E:404:ASN:HA	1:E:407:PHE:CE2	2.46	0.50
1:F:127:PRO:HG2	1:F:293:GLU:HA	1.92	0.50
1:D:154:VAL:HG21	1:D:167:GLU:HG3	1.92	0.50
1:D:404:ASN:HA	1:D:407:PHE:CE2	2.46	0.50
1:E:132:ASP:O	1:E:135:ILE:HD11	2.10	0.50
1:E:127:PRO:HG2	1:E:293:GLU:HA	1.92	0.50
1:E:20:ASN:HD22	1:E:417:ASP:HB2	1.77	0.50
1:C:339:ASN:ND2	1:C:342:TYR:H	2.06	0.50
1:E:312:PHE:O	1:E:328:SER:HA	2.12	0.50
1:A:151:ALA:HB2	1:A:190:ILE:CD1	2.23	0.50
1:F:191:THR:HA	2:F:606:MYA:HEMA	1.93	0.50
1:C:382:TYR:O	1:C:386:ILE:HD12	2.12	0.50
1:A:165:SER:HB3	1:A:201:HIS:HB2	1.93	0.50
1:E:229:LEU:HB3	1:E:235:THR:HG22	1.94	0.49
1:C:211:PRO:O	1:C:212:ALA:CB	2.60	0.49
1:E:269:ILE:HD13	1:E:295:GLU:HB2	1.93	0.49
1:D:155:THR:HG22	1:D:288:ILE:HD12	1.93	0.49
1:D:68:ILE:O	1:D:196:LYS:HE2	2.12	0.49
1:D:22:ASP:HB2	1:D:26:LYS:HB2	1.94	0.49
1:D:135:ILE:HG22	1:D:136:GLY:N	2.28	0.49
1:C:95:VAL:O	1:C:99:LEU:HD23	2.12	0.49
1:E:202:ALA:HB2	2:E:605:MYA:HEM	1.94	0.49
1:C:315:VAL:HG22	1:C:323:ILE:HG23	1.93	0.49
1:C:232:VAL:HG12	1:C:232:VAL:O	2.12	0.49
1:F:336:ILE:CD1	1:F:345:LEU:HB2	2.37	0.49
1:D:208:ILE:H	1:D:208:ILE:HD12	1.78	0.49
1:E:439:ASP:O	1:E:440:ASN:HB2	2.12	0.49
1:F:311:ILE:HD13	1:F:312:PHE:H	1.77	0.49
1:D:181:ARG:HG3	1:D:184:PRO:HG2	1.94	0.49
1:E:339:ASN:ND2	1:E:342:TYR:N	2.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:LEU:HD22	1:E:172:CYS:HB2	1.95	0.48
1:F:60:ASP:H	1:F:426:ASN:HD21	1.60	0.48
1:A:168:ILE:HG22	2:A:601:MYA:H3MA	1.95	0.48
1:D:68:ILE:HG22	1:D:196:LYS:HG2	1.96	0.48
1:C:227:LYS:HD3	1:C:247:ILE:HD11	1.95	0.48
1:E:107:ARG:HH11	1:E:175:LYS:HZ2	1.59	0.48
1:B:99:LEU:O	1:B:103:TYR:HB2	2.13	0.48
1:B:99:LEU:HD13	1:B:103:TYR:CE1	2.49	0.48
1:B:328:SER:OG	1:B:351:TYR:HB3	2.13	0.48
1:F:187:ILE:O	1:F:190:ILE:HG22	2.14	0.48
1:E:232:VAL:O	1:E:232:VAL:CG1	2.61	0.48
1:F:187:ILE:HG12	2:F:606:MYA:H7M	1.95	0.48
1:A:232:VAL:HG12	1:A:232:VAL:O	2.13	0.48
1:E:174:HIS:CD2	1:E:176:GLN:H	2.32	0.48
1:D:106:ASP:HB3	1:D:109:ALA:HB2	1.96	0.48
1:A:272:VAL:HG22	1:A:323:ILE:HG21	1.94	0.48
1:F:174:HIS:CD2	1:F:176:GLN:H	2.32	0.47
1:C:202:ALA:HB3	1:C:425:PHE:HB3	1.95	0.47
1:B:315:VAL:HG22	1:B:323:ILE:HG23	1.96	0.47
1:A:191:THR:HA	2:A:601:MYA:HDMA	1.96	0.47
1:A:39:LYS:HG2	1:A:181:ARG:NH2	2.28	0.47
1:C:58:PRO:HG3	1:C:201:HIS:HE1	1.79	0.47
1:D:127:PRO:HG2	1:D:293:GLU:CA	2.44	0.47
1:C:61:LYS:N	1:C:61:LYS:HD3	2.28	0.47
1:F:252:LEU:HD21	1:F:385:CYS:HB3	1.97	0.47
1:B:217:CYS:HB3	1:B:399:LEU:O	2.14	0.47
1:E:45:PRO:HB2	1:E:426:ASN:HD22	1.79	0.47
1:C:432:ILE:CG2	1:C:449:ASN:HB2	2.44	0.47
1:A:12:ASN:O	1:A:16:LEU:HG	2.14	0.47
1:A:405:THR:HG21	1:A:443:ASP:C	2.34	0.47
1:A:191:THR:HG23	2:A:601:MYA:HEM	1.97	0.47
1:F:242:THR:HG22	1:F:244:GLU:N	2.27	0.47
1:F:194:VAL:O	1:F:197:CYS:N	2.48	0.47
1:C:149:ILE:HD12	1:C:171:LEU:HD13	1.95	0.47
1:C:269:ILE:HG13	1:C:295:GLU:HG3	1.97	0.47
1:B:220:THR:HG22	1:B:415:PRO:HA	1.96	0.47
1:A:187:ILE:HG12	2:A:601:MYA:H7MA	1.97	0.47
1:C:408:LEU:O	1:C:413:PHE:HB2	2.15	0.47
1:F:58:PRO:O	1:F:428:ARG:NH1	2.46	0.47
1:B:38:HIS:HA	2:B:602:MYA:P3X	2.55	0.47
1:B:373:LEU:HD22	1:B:377:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:VAL:HB	1:E:177:LEU:HD21	1.96	0.47
1:E:187:ILE:HG23	2:E:605:MYA:H9M	1.97	0.46
1:C:187:ILE:O	1:C:190:ILE:HG22	2.15	0.46
1:E:106:ASP:HB3	1:E:109:ALA:HB2	1.96	0.46
1:C:138:ARG:NH1	1:C:143:GLN:O	2.43	0.46
1:D:232:VAL:O	1:D:232:VAL:CG1	2.64	0.46
1:C:432:ILE:HG23	1:C:449:ASN:HB2	1.96	0.46
1:A:93:GLU:HA	1:A:96:PHE:CZ	2.50	0.46
1:E:337:LEU:O	1:E:339:ASN:N	2.40	0.46
1:A:22:ASP:OD1	1:A:22:ASP:N	2.49	0.46
1:D:263:LYS:HD3	1:D:263:LYS:N	2.29	0.46
1:A:21:ASN:O	1:A:22:ASP:C	2.53	0.46
1:E:283:PHE:CE2	1:E:402:GLN:HA	2.50	0.46
1:A:39:LYS:HG2	1:A:181:ARG:HH22	1.79	0.46
1:F:165:SER:HB3	1:F:201:HIS:HB2	1.98	0.46
1:B:106:ASP:HB3	1:B:109:ALA:HB2	1.97	0.46
1:A:406:LEU:HD21	1:A:447:ARG:HH11	1.80	0.46
1:E:40:PHE:CD1	1:E:184:PRO:HB3	2.51	0.46
1:D:271:GLN:HB3	1:D:323:ILE:HD12	1.97	0.46
1:F:86:VAL:HG13	1:F:92:LEU:HD13	1.98	0.46
1:C:252:LEU:HD21	1:C:385:CYS:HB3	1.98	0.46
1:B:401:SER:O	1:B:404:ASN:HB2	2.16	0.45
1:C:388:ALA:O	1:C:393:MET:HG2	2.16	0.45
1:D:149:ILE:HD12	1:D:171:LEU:HD13	1.98	0.45
1:E:205:THR:CG2	1:E:454:MET:HG3	2.46	0.45
1:D:243:GLU:O	1:D:247:ILE:HG12	2.16	0.45
1:A:98:LEU:HD22	1:A:145:LEU:HG	1.98	0.45
1:A:166:VAL:HG13	1:A:168:ILE:HD12	1.98	0.45
1:E:171:LEU:HB3	2:E:605:MYA:H3A	1.99	0.45
1:B:132:ASP:O	1:B:135:ILE:HD11	2.17	0.45
1:E:262:ARG:HH21	1:E:317:GLU:HB2	1.82	0.45
1:E:56:GLU:HG2	1:E:429:ALA:HA	1.99	0.45
1:B:324:THR:HG23	1:B:356:ASP:OD1	2.16	0.45
1:A:242:THR:HG22	1:A:244:GLU:N	2.31	0.45
1:C:393:MET:HB3	1:C:393:MET:HE2	1.92	0.45
1:D:324:THR:HG22	1:D:325:ASP:OD2	2.16	0.45
1:D:25:SER:HA	1:D:105:GLU:HB2	1.98	0.45
1:B:98:LEU:HD22	1:B:145:LEU:HG	1.97	0.45
1:C:165:SER:HB3	1:C:201:HIS:HB2	1.99	0.45
1:C:25:SER:HB2	1:C:104:VAL:HA	1.99	0.45
1:A:210:LEU:HB3	1:A:211:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:GLN:NE2	1:D:421:ASN:HD21	2.15	0.44
1:C:156:LEU:HD11	1:C:203:LEU:HB2	1.98	0.44
1:B:147:ALA:HA	1:B:172:CYS:O	2.17	0.44
1:D:210:LEU:O	1:D:213:PRO:HD3	2.16	0.44
1:E:107:ARG:HD2	1:E:175:LYS:HZ3	1.83	0.44
1:C:324:THR:HG23	1:C:356:ASP:OD1	2.17	0.44
1:A:278:ARG:HG3	1:A:278:ARG:HH11	1.82	0.44
1:B:437:ASN:HD21	1:B:445:LYS:HE3	1.81	0.44
1:B:339:ASN:ND2	1:B:342:TYR:H	2.13	0.44
1:F:127:PRO:HD3	1:F:296:HIS:CD2	2.53	0.44
1:F:363:ASP:HB2	1:F:366:ASP:HB2	2.00	0.44
1:D:191:THR:HA	2:D:604:MYA:HEMA	2.00	0.44
1:F:130:LYS:HG3	1:F:132:ASP:HB2	2.00	0.44
1:A:126:SER:O	1:A:129:TRP:HB3	2.17	0.44
1:B:361:PHE:HE2	1:B:368:LYS:HG3	1.81	0.44
1:B:47:LYS:HD2	1:B:212:ALA:CB	2.31	0.44
1:F:117:LYS:O	1:F:121:ASN:HB2	2.18	0.44
1:B:88:ASN:HD22	1:B:88:ASN:C	2.20	0.44
1:D:56:GLU:HG2	1:D:429:ALA:HA	2.00	0.44
1:F:166:VAL:O	1:F:202:ALA:HA	2.18	0.43
1:E:269:ILE:HD11	1:E:299:ILE:HD13	1.99	0.43
1:A:404:ASN:HA	1:A:407:PHE:CE2	2.53	0.43
1:C:59:ILE:H	1:C:426:ASN:ND2	2.15	0.43
1:A:211:PRO:O	1:A:212:ALA:CB	2.67	0.43
1:A:45:PRO:O	1:A:426:ASN:HA	2.18	0.43
1:A:87:ASP:OD2	1:A:125:LYS:HE2	2.19	0.43
1:A:399:LEU:C	1:A:401:SER:H	2.22	0.43
1:E:346:GLY:HA3	1:E:393:MET:HA	2.01	0.43
1:B:187:ILE:HG23	2:B:602:MYA:H9M	2.01	0.43
1:E:71:LYS:O	1:E:71:LYS:HG2	2.18	0.43
1:B:6:LYS:O	1:B:10:LEU:HD12	2.19	0.43
1:A:53:VAL:HG13	1:A:430:LYS:HG2	2.00	0.43
1:E:202:ALA:HB3	1:E:425:PHE:HB3	2.01	0.43
2:B:602:MYA:H12A	2:B:602:MYA:N7A	2.34	0.43
1:B:135:ILE:HD11	1:B:193:ARG:HD2	2.01	0.43
1:C:181:ARG:NH2	2:C:603:MYA:O7A	2.52	0.43
1:C:232:VAL:CG1	1:C:232:VAL:O	2.67	0.43
1:D:86:VAL:HG13	1:D:92:LEU:HD13	2.01	0.43
1:B:382:TYR:O	1:B:386:ILE:HD12	2.18	0.43
1:C:192:ARG:HH11	1:C:192:ARG:HG2	1.84	0.43
1:A:405:THR:HG21	1:A:444:ILE:HA	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:GLY:O	1:C:153:PRO:HG3	2.19	0.43
1:D:98:LEU:HD22	1:D:145:LEU:HG	2.01	0.43
1:E:149:ILE:HD11	1:E:168:ILE:CG2	2.48	0.43
1:A:166:VAL:O	1:A:202:ALA:HA	2.19	0.43
1:C:168:ILE:HG22	2:C:603:MYA:H3MA	2.00	0.43
1:A:408:LEU:O	1:A:413:PHE:HB2	2.18	0.43
1:D:229:LEU:HD21	1:D:395:VAL:HB	2.01	0.43
1:E:345:LEU:HD12	1:E:394:ASP:OD1	2.19	0.42
1:A:127:PRO:HG2	1:A:293:GLU:CA	2.49	0.42
1:E:111:PHE:HA	1:E:335:THR:O	2.19	0.42
1:F:135:ILE:HD11	1:F:190:ILE:HD13	2.01	0.42
1:F:53:VAL:HG21	1:F:428:ARG:HB3	2.00	0.42
1:F:174:HIS:HB3	1:F:177:LEU:HD21	2.01	0.42
1:E:20:ASN:ND2	1:E:417:ASP:O	2.52	0.42
1:A:406:LEU:HG	1:A:447:ARG:HD2	2.00	0.42
1:A:373:LEU:HD22	1:A:377:LEU:HG	2.01	0.42
1:B:405:THR:HG21	1:B:447:ARG:HA	2.02	0.42
1:D:357:ALA:HB2	1:D:376:ARG:HG2	2.01	0.42
1:A:180:LYS:HD3	1:A:180:LYS:HA	1.91	0.42
1:D:373:LEU:HD22	1:D:377:LEU:HG	2.00	0.42
1:F:286:ILE:HG22	1:F:451:GLY:HA3	2.02	0.42
1:F:40:PHE:HE1	1:F:188:LYS:HE3	1.84	0.42
1:A:278:ARG:HD2	1:A:359:PHE:CZ	2.55	0.42
1:E:68:ILE:HD11	1:E:200:TRP:HH2	1.78	0.42
1:E:205:THR:O	1:E:206:ALA:HB2	2.20	0.42
1:A:266:LYS:HD2	1:A:269:ILE:HD12	2.02	0.42
1:F:133:TRP:HH2	1:F:199:ILE:HD12	1.85	0.42
1:F:84:ILE:HG12	1:F:95:VAL:CG2	2.50	0.42
1:B:40:PHE:CD1	1:B:184:PRO:HB3	2.55	0.41
1:A:45:PRO:HB3	1:A:426:ASN:HD22	1.85	0.41
1:E:177:LEU:O	1:E:180:LYS:HG2	2.21	0.41
1:A:149:ILE:HD12	1:A:171:LEU:HD13	2.01	0.41
1:A:44:GLN:HA	1:A:45:PRO:HD3	1.87	0.41
1:C:64:THR:HG23	1:C:66:GLU:HB3	2.01	0.41
2:C:603:MYA:H6MA	2:C:603:MYA:H2AA	2.02	0.41
1:D:331:SER:HB2	1:D:393:MET:HE3	2.02	0.41
1:D:298:PHE:HA	1:D:311:ILE:HD12	2.02	0.41
1:C:44:GLN:HA	1:C:45:PRO:HD3	1.83	0.41
1:B:71:LYS:HG2	1:B:71:LYS:O	2.20	0.41
1:A:159:ARG:HG3	1:A:284:GLU:HB3	2.02	0.41
1:F:277:LYS:NZ	1:F:289:PHE:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ILE:O	1:D:194:VAL:HG23	2.20	0.41
1:B:142:THR:O	1:B:143:GLN:HB2	2.21	0.41
1:B:337:LEU:O	1:B:339:ASN:N	2.45	0.41
1:B:174:HIS:CD2	1:B:176:GLN:HB2	2.55	0.41
1:F:98:LEU:HD22	1:F:145:LEU:HG	2.03	0.41
1:D:212:ALA:H	1:D:213:PRO:HD3	1.85	0.41
1:B:293:GLU:O	1:B:297:ASN:HB2	2.21	0.41
1:F:318:GLN:HB3	1:F:319:PRO:HD2	2.03	0.41
1:C:221:HIS:ND1	1:C:397:ASN:ND2	2.68	0.41
1:C:229:LEU:HB3	1:C:235:THR:HG22	2.03	0.41
1:B:262:ARG:HH21	1:B:317:GLU:HB2	1.85	0.41
1:C:286:ILE:HG22	1:C:451:GLY:HA3	2.03	0.41
1:F:210:LEU:HB3	1:F:211:PRO:HD2	2.03	0.41
1:E:73:LEU:HA	1:E:74:PRO:HD3	1.89	0.41
1:B:339:ASN:HD22	1:B:341:LYS:N	2.16	0.40
1:F:202:ALA:CB	2:F:606:MYA:HDMA	2.45	0.40
2:B:602:MYA:N8	2:B:602:MYA:O5	2.53	0.40
1:B:232:VAL:O	1:B:232:VAL:CG1	2.68	0.40
1:D:232:VAL:O	1:D:232:VAL:HG12	2.20	0.40
1:C:403:ASP:OD2	1:C:447:ARG:HD2	2.20	0.40
1:B:68:ILE:HG13	1:B:195:ASN:HB3	2.03	0.40
1:D:278:ARG:HD2	1:D:359:PHE:CZ	2.55	0.40
1:E:149:ILE:HD12	1:E:190:ILE:HG21	2.04	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	438/455 (96%)	400 (91%)	31 (7%)	7 (2%)	12 40
1	B	439/455 (96%)	410 (93%)	24 (6%)	5 (1%)	17 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	442/455 (97%)	390 (88%)	47 (11%)	5 (1%)	17	51
1	D	439/455 (96%)	399 (91%)	33 (8%)	7 (2%)	12	40
1	E	439/455 (96%)	407 (93%)	29 (7%)	3 (1%)	26	63
1	F	434/455 (95%)	387 (89%)	42 (10%)	5 (1%)	16	48
All	All	2631/2730 (96%)	2393 (91%)	206 (8%)	32 (1%)	16	48

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ALA
1	C	212	ALA
1	D	77	SER
1	D	212	ALA
1	F	212	ALA
1	A	78	SER
1	A	281	SER
1	A	400	THR
1	B	78	SER
1	C	21	ASN
1	C	78	SER
1	E	78	SER
1	E	338	ASN
1	F	196	LYS
1	A	22	ASP
1	C	192	ARG
1	D	303	SER
1	B	337	LEU
1	B	338	ASN
1	D	22	ASP
1	D	337	LEU
1	E	211	PRO
1	B	211	PRO
1	F	78	SER
1	F	338	ASN
1	D	211	PRO
1	C	65	PRO
1	D	438	PRO
1	A	213	PRO
1	A	438	PRO
1	B	269	ILE
1	F	62	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	400/413 (97%)	369 (92%)	31 (8%)	16	41
1	B	401/413 (97%)	359 (90%)	42 (10%)	8	25
1	C	404/413 (98%)	370 (92%)	34 (8%)	14	37
1	D	401/413 (97%)	371 (92%)	30 (8%)	17	44
1	E	401/413 (97%)	368 (92%)	33 (8%)	14	39
1	F	396/413 (96%)	371 (94%)	25 (6%)	22	54
All	All	2403/2478 (97%)	2208 (92%)	195 (8%)	15	39

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	19	LEU
1	A	21	ASN
1	A	53	VAL
1	A	66	GLU
1	A	70	ASP
1	A	84	ILE
1	A	99	LEU
1	A	108	ASP
1	A	112	ARG
1	A	126	SER
1	A	165	SER
1	A	166	VAL
1	A	177	LEU
1	A	190	ILE
1	A	198	ASP
1	A	242	THR
1	A	252	LEU
1	A	278	ARG
1	A	311	ILE
1	A	315	VAL
1	A	326	PHE

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Mol	Chain	Res	Type
1	A	332	LEU
1	A	338	ASN
1	A	339	ASN
1	A	344	ASP
1	A	347	ILE
1	A	373	LEU
1	A	393	MET
1	A	417	ASP
1	A	420	LEU
1	B	10	LEU
1	B	37	ASP
1	B	47	LYS
1	B	53	VAL
1	B	66	GLU
1	B	73	LEU
1	B	77	SER
1	B	88	ASN
1	B	99	LEU
1	B	103	TYR
1	B	105	GLU
1	B	131	LYS
1	B	166	VAL
1	B	168	ILE
1	B	177	LEU
1	B	208	ILE
1	B	242	THR
1	B	261	LEU
1	B	270	ASP
1	B	271	GLN
1	B	278	ARG
1	B	295	GLU
1	B	297	ASN
1	B	306	LEU
1	B	307	ASP
1	B	332	LEU
1	B	338	ASN
1	B	339	ASN
1	B	340	THR
1	B	351	TYR
1	B	355	THR
1	B	362	LYS
1	B	371	LYS

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Mol	Chain	Res	Type
1	B	373	LEU
1	B	405	THR
1	B	410	ASP
1	B	412	LYS
1	B	420	LEU
1	B	439	ASP
1	B	444	ILE
1	B	445	LYS
1	B	452	VAL
1	C	5	ASP
1	C	6	LYS
1	C	13	LEU
1	C	61	LYS
1	C	99	LEU
1	C	112	ARG
1	C	121	ASN
1	C	125	LYS
1	C	135	ILE
1	C	155	THR
1	C	198	ASP
1	C	201	HIS
1	C	222	ARG
1	C	252	LEU
1	C	261	LEU
1	C	278	ARG
1	C	311	ILE
1	C	315	VAL
1	C	326	PHE
1	C	332	LEU
1	C	338	ASN
1	C	344	ASP
1	C	351	TYR
1	C	362	LYS
1	C	371	LYS
1	C	373	LEU
1	C	375	THR
1	C	393	MET
1	C	410	ASP
1	C	420	LEU
1	C	426	ASN
1	C	444	ILE
1	C	445	LYS

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Mol	Chain	Res	Type
1	C	452	VAL
1	D	13	LEU
1	D	27	PHE
1	D	53	VAL
1	D	73	LEU
1	D	76	LEU
1	D	96	PHE
1	D	112	ARG
1	D	130	LYS
1	D	162	GLN
1	D	166	VAL
1	D	177	LEU
1	D	242	THR
1	D	252	LEU
1	D	263	LYS
1	D	278	ARG
1	D	311	ILE
1	D	315	VAL
1	D	332	LEU
1	D	339	ASN
1	D	343	LYS
1	D	344	ASP
1	D	362	LYS
1	D	368	LYS
1	D	371	LYS
1	D	373	LEU
1	D	405	THR
1	D	420	LEU
1	D	430	LYS
1	D	445	LYS
1	D	446	ARG
1	E	6	LYS
1	E	10	LEU
1	E	17	LEU
1	E	25	SER
1	E	28	THR
1	E	53	VAL
1	E	70	ASP
1	E	73	LEU
1	E	88	ASN
1	E	103	TYR
1	E	105	GLU

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Mol	Chain	Res	Type
1	E	149	ILE
1	E	152	ILE
1	E	166	VAL
1	E	177	LEU
1	E	208	ILE
1	E	234	PHE
1	E	242	THR
1	E	252	LEU
1	E	271	GLN
1	E	278	ARG
1	E	295	GLU
1	E	332	LEU
1	E	340	THR
1	E	362	LYS
1	E	371	LYS
1	E	373	LEU
1	E	399	LEU
1	E	405	THR
1	E	410	ASP
1	E	420	LEU
1	E	445	LYS
1	E	452	VAL
1	F	88	ASN
1	F	99	LEU
1	F	107	ARG
1	F	149	ILE
1	F	177	LEU
1	F	190	ILE
1	F	208	ILE
1	F	261	LEU
1	F	263	LYS
1	F	270	ASP
1	F	286	ILE
1	F	291	LYS
1	F	295	GLU
1	F	302	GLU
1	F	311	ILE
1	F	315	VAL
1	F	332	LEU
1	F	339	ASN
1	F	373	LEU
1	F	386	ILE

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Mol	Chain	Res	Type
1	F	393	MET
1	F	399	LEU
1	F	420	LEU
1	F	452	VAL
1	F	454	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	A	176	GLN
1	A	195	ASN
1	A	339	ASN
1	A	397	ASN
1	A	404	ASN
1	A	421	ASN
1	A	426	ASN
1	B	20	ASN
1	B	88	ASN
1	B	114	ASN
1	B	174	HIS
1	B	195	ASN
1	B	339	ASN
1	B	397	ASN
1	B	404	ASN
1	B	421	ASN
1	B	426	ASN
1	B	437	ASN
1	C	29	GLN
1	C	114	ASN
1	C	174	HIS
1	C	195	ASN
1	C	201	HIS
1	C	338	ASN
1	C	339	ASN
1	C	397	ASN
1	C	404	ASN
1	C	421	ASN
1	C	426	ASN
1	D	20	ASN
1	D	162	GLN
1	D	174	HIS

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Mol	Chain	Res	Type
1	D	297	ASN
1	D	339	ASN
1	D	392	ASN
1	D	397	ASN
1	D	421	ASN
1	D	426	ASN
1	D	437	ASN
1	E	18	GLN
1	E	20	ASN
1	E	88	ASN
1	E	174	HIS
1	E	195	ASN
1	E	297	ASN
1	E	339	ASN
1	E	397	ASN
1	E	404	ASN
1	E	426	ASN
1	E	437	ASN
1	F	88	ASN
1	F	162	GLN
1	F	174	HIS
1	F	195	ASN
1	F	201	HIS
1	F	241	HIS
1	F	296	HIS
1	F	339	ASN
1	F	397	ASN
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

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MYA	A	601	-	53,65,65	1.19	5 (9%)	65,91,91	1.78	6 (9%)
2	MYA	B	602	-	53,65,65	1.20	5 (9%)	65,91,91	1.84	8 (12%)
2	MYA	C	603	-	53,65,65	1.22	5 (9%)	65,91,91	1.74	5 (7%)
2	MYA	D	604	-	53,65,65	1.23	5 (9%)	65,91,91	1.81	6 (9%)
2	MYA	E	605	-	53,65,65	1.10	5 (9%)	65,91,91	1.84	8 (12%)
2	MYA	F	606	-	53,65,65	1.22	5 (9%)	65,91,91	1.74	5 (7%)

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
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

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	605	MYA	O4X-C1X	2.01	1.43	1.41
2	C	603	MYA	P3X-O8A	2.04	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	606	MYA	P3X-O8A	2.13	1.62	1.54
2	B	602	MYA	P3X-O8A	2.20	1.62	1.54
2	E	605	MYA	P3X-O8A	2.22	1.62	1.54
2	A	601	MYA	P3X-O8A	2.29	1.62	1.54
2	D	604	MYA	P3X-O8A	2.35	1.63	1.54
2	B	602	MYA	P1A-O2A	2.84	1.61	1.51
2	F	606	MYA	P1A-O2A	2.92	1.61	1.51
2	A	601	MYA	P1A-O2A	2.92	1.61	1.51
2	D	604	MYA	P1A-O2A	2.97	1.62	1.51
2	E	605	MYA	P1A-O2A	3.12	1.62	1.51
2	C	603	MYA	P1A-O2A	3.19	1.62	1.51
2	A	601	MYA	P3X-O9A	3.28	1.61	1.51
2	F	606	MYA	P3X-O9A	3.31	1.62	1.51
2	E	605	MYA	P3X-O9A	3.32	1.62	1.51
2	D	604	MYA	P3X-O9A	3.34	1.62	1.51
2	A	601	MYA	P2A-O4A	3.35	1.63	1.51
2	C	603	MYA	P3X-O9A	3.36	1.62	1.51
2	B	602	MYA	P3X-O9A	3.38	1.62	1.51
2	E	605	MYA	P2A-O4A	3.41	1.63	1.51
2	D	604	MYA	P2A-O4A	3.46	1.63	1.51
2	B	602	MYA	P2A-O4A	3.48	1.63	1.51
2	C	603	MYA	P2A-O4A	3.61	1.64	1.51
2	F	606	MYA	O4X-C1X	3.64	1.45	1.41
2	B	602	MYA	O4X-C1X	3.66	1.45	1.41
2	A	601	MYA	O4X-C1X	3.71	1.45	1.41
2	F	606	MYA	P2A-O4A	3.75	1.64	1.51
2	C	603	MYA	O4X-C1X	3.77	1.46	1.41
2	D	604	MYA	O4X-C1X	3.79	1.46	1.41

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	606	MYA	N3A-C2A-N1A	-9.56	121.57	128.89
2	B	602	MYA	N3A-C2A-N1A	-9.53	121.60	128.89
2	A	601	MYA	N3A-C2A-N1A	-9.53	121.60	128.89
2	D	604	MYA	N3A-C2A-N1A	-9.51	121.61	128.89
2	C	603	MYA	N3A-C2A-N1A	-9.33	121.75	128.89
2	E	605	MYA	N3A-C2A-N1A	-9.32	121.76	128.89
2	D	604	MYA	P2A-O3A-P1A	-3.85	121.93	132.73
2	B	602	MYA	P2A-O3A-P1A	-3.70	122.35	132.73
2	F	606	MYA	P2A-O3A-P1A	-3.68	122.39	132.73
2	E	605	MYA	P2A-O3A-P1A	-3.56	122.74	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	MYA	P2A-O3A-P1A	-3.24	123.63	132.73
2	B	602	MYA	C6-C7-N8	-2.95	105.40	111.88
2	A	601	MYA	C2X-C1X-N9A	-2.75	110.10	114.29
2	B	602	MYA	C10-C9-N8	-2.72	110.45	116.47
2	C	603	MYA	P2A-O3A-P1A	-2.64	125.31	132.73
2	E	605	MYA	C6-C7-N8	-2.46	106.48	111.88
2	E	605	MYA	C2-C3-N4	-2.34	107.68	112.36
2	D	604	MYA	C4A-C5A-N7A	-2.33	107.34	109.48
2	E	605	MYA	C4A-C5A-N7A	-2.32	107.34	109.48
2	B	602	MYA	C4A-C5A-N7A	-2.31	107.35	109.48
2	E	605	MYA	C4X-O4X-C1X	-2.26	107.23	109.72
2	D	604	MYA	C2X-C1X-N9A	-2.11	111.08	114.29
2	C	603	MYA	C4A-C5A-N7A	-2.04	107.60	109.48
2	A	601	MYA	C4A-C5A-N7A	-2.04	107.60	109.48
2	F	606	MYA	C4A-C5A-N7A	-2.04	107.61	109.48
2	B	602	MYA	C14-C11-C10	2.01	113.02	109.34
2	E	605	MYA	O3A-P2A-O6A	2.92	110.68	102.94
2	B	602	MYA	O3A-P2A-O6A	2.93	110.70	102.94
2	F	606	MYA	O3A-P2A-O6A	3.06	111.04	102.94
2	A	601	MYA	O3A-P2A-O6A	3.63	112.56	102.94
2	D	604	MYA	O3A-P2A-O6A	3.64	112.59	102.94
2	C	603	MYA	O3A-P2A-O6A	3.83	113.09	102.94
2	D	604	MYA	O2M-C2M-C3M	6.05	120.11	109.05
2	A	601	MYA	O2M-C2M-C3M	6.09	120.19	109.05
2	B	602	MYA	O2M-C2M-C3M	6.10	120.21	109.05
2	F	606	MYA	O2M-C2M-C3M	6.14	120.28	109.05
2	C	603	MYA	O2M-C2M-C3M	6.25	120.49	109.05
2	E	605	MYA	O2M-C2M-C3M	6.81	121.52	109.05

All (6) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	MYA	7	0
2	B	602	MYA	5	0
2	C	603	MYA	6	0
2	D	604	MYA	2	0
2	E	605	MYA	8	0
2	F	606	MYA	5	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	442/455 (97%)	-0.01	11 (2%) 61 55	28, 45, 73, 95	0
1	B	443/455 (97%)	-0.10	5 (1%) 82 80	29, 44, 71, 92	0
1	C	446/455 (98%)	0.09	11 (2%) 61 55	29, 55, 82, 102	0
1	D	443/455 (97%)	-0.08	7 (1%) 74 72	29, 45, 69, 110	0
1	E	443/455 (97%)	-0.11	7 (1%) 74 72	26, 41, 67, 93	0
1	F	438/455 (96%)	0.16	7 (1%) 74 72	35, 60, 92, 119	0
All	All	2655/2730 (97%)	-0.01	48 (1%) 71 68	26, 48, 80, 119	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	27	PHE	5.3
1	B	27	PHE	5.2
1	E	27	PHE	4.8
1	A	27	PHE	4.2
1	B	24	THR	4.2
1	B	25	SER	4.0
1	C	37	ASP	4.0
1	F	39	LYS	3.8
1	E	24	THR	3.7
1	C	24	THR	3.4
1	F	24	THR	3.4
1	E	25	SER	3.3
1	B	23	ASP	3.3
1	D	26	LYS	3.3
1	D	27	PHE	3.2
1	A	25	SER	3.1
1	C	26	LYS	2.7
1	A	26	LYS	2.7
1	C	23	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	42	ARG	2.5
1	C	212	ALA	2.5
1	E	50	ASP	2.5
1	E	28	THR	2.4
1	A	303	SER	2.4
1	C	6	LYS	2.4
1	C	39	LYS	2.3
1	C	29	GLN	2.3
1	A	23	ASP	2.3
1	A	39	LYS	2.3
1	D	36	LYS	2.3
1	F	79	PHE	2.2
1	A	37	ASP	2.2
1	F	23	ASP	2.2
1	C	41	TRP	2.2
1	A	24	THR	2.2
1	C	66	GLU	2.1
1	A	338	ASN	2.1
1	F	71	LYS	2.1
1	F	49	PHE	2.1
1	D	22	ASP	2.1
1	A	179	SER	2.1
1	F	78	SER	2.1
1	D	37	ASP	2.1
1	D	24	THR	2.1
1	E	5	ASP	2.0
1	B	28	THR	2.0
1	D	61	LYS	2.0
1	E	26	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MYA	C	603	63/63	0.84	0.28	0.32	68,78,82,85	0
2	MYA	F	606	63/63	0.88	0.25	0.12	74,80,83,83	0
2	MYA	D	604	63/63	0.87	0.22	0.04	47,62,79,80	0
2	MYA	B	602	63/63	0.90	0.21	-0.01	31,66,72,73	0
2	MYA	E	605	63/63	0.90	0.20	-0.21	32,57,62,62	0
2	MYA	A	601	63/63	0.87	0.21	-0.38	51,65,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.