



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 07:46 pm BST

PDB ID : 3BWN
Title : L-tryptophan aminotransferase
Authors : Ferrer, J.-L.; Noel, J.P.; Pojer, F.; Bowman, M.; Chory, J.; Tao, Y.
Deposited on : 2008-01-10
Resolution : 2.25 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

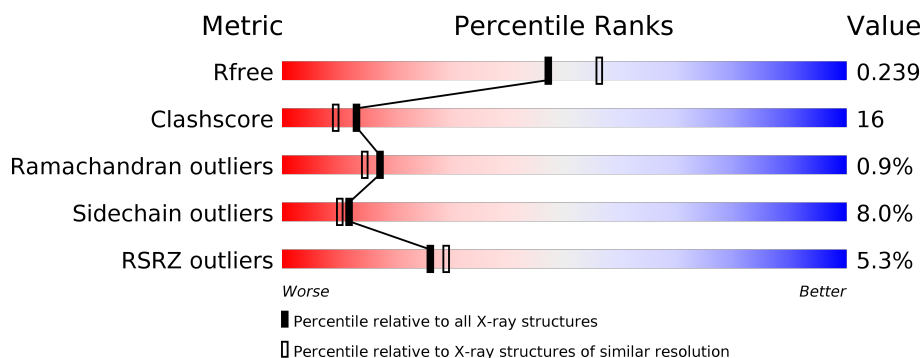
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 respectively. 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	391	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	391	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>23%</div> <div>•</div> <div>6%</div> </div> </div>
1	D	391	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>24%</div> <div>•</div> <div>8%</div> </div> </div>
1	E	391	<div> <div>8%</div> <div> <div></div> <div>57%</div> <div>27%</div> <div>8%</div> <div>•</div> <div>7%</div> </div> </div>
1	F	391	<div> <div>6%</div> <div> <div></div> <div>60%</div> <div>29%</div> <div>• •</div> <div>8%</div> </div> </div>
2	C	391	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>24%</div> <div>5%</div> <div>8%</div> </div> </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
3	PMP	A	1001	-	-	X	-
3	PMP	B	1001	-	-	X	-
3	PMP	F	1001[A]	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18137 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.

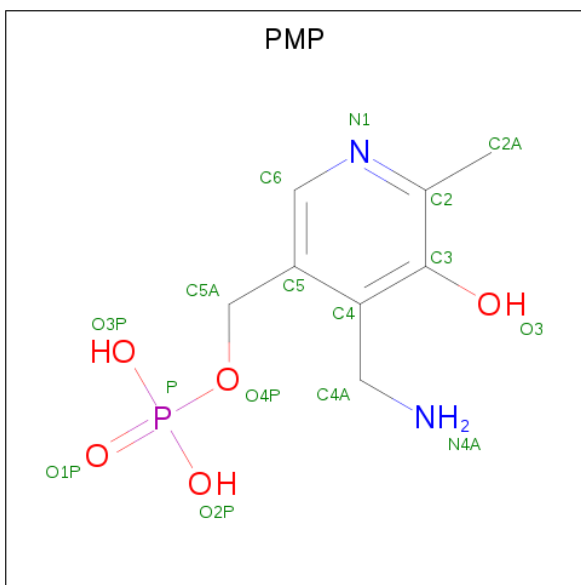
- Molecule 1 is a protein called L-tryptophan aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2906	1848	494	545	19			
1	B	369	Total	C	N	O	S	0	0	0
			2962	1878	505	560	19			
1	D	359	Total	C	N	O	S	0	1	0
			2886	1833	491	543	19			
1	E	362	Total	C	N	O	S	0	0	0
			2900	1847	491	543	19			
1	F	360	Total	C	N	O	S	0	1	0
			2892	1840	492	541	19			

- Molecule 2 is a protein called L-tryptophan aminotransferase.

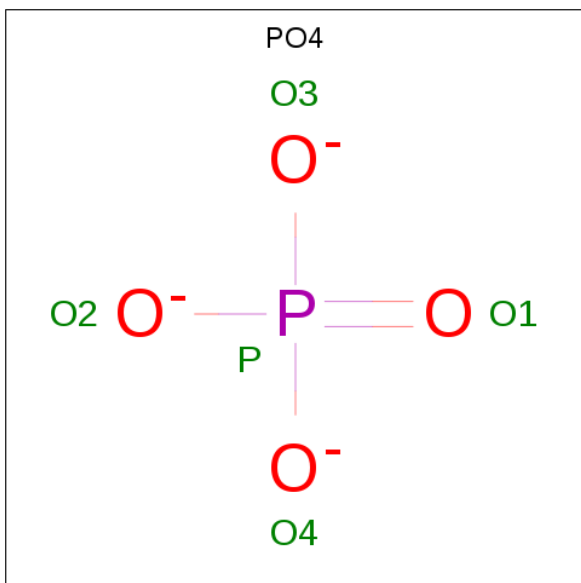
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	361	Total	C	N	O	P S	0	0	0
			2918	1855	494	549	1 19			

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).



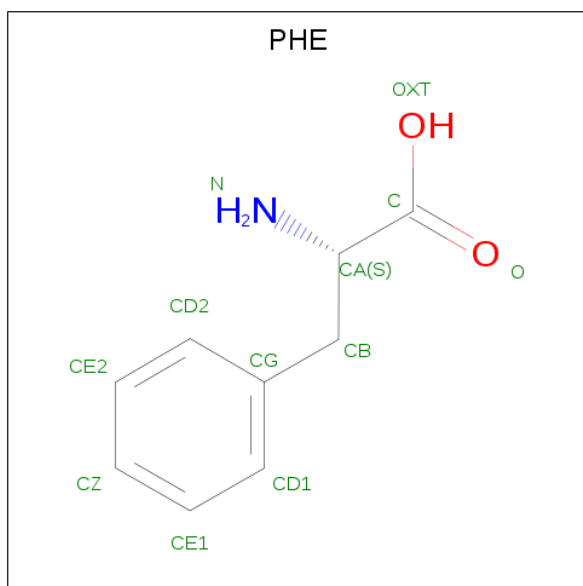
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	D	1	Total	C	N	O	P	0	1
			16	8	2	5	1		
3	F	1	Total	C	N	O	P	0	1
			16	8	2	5	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	1
			12	9	1	2		

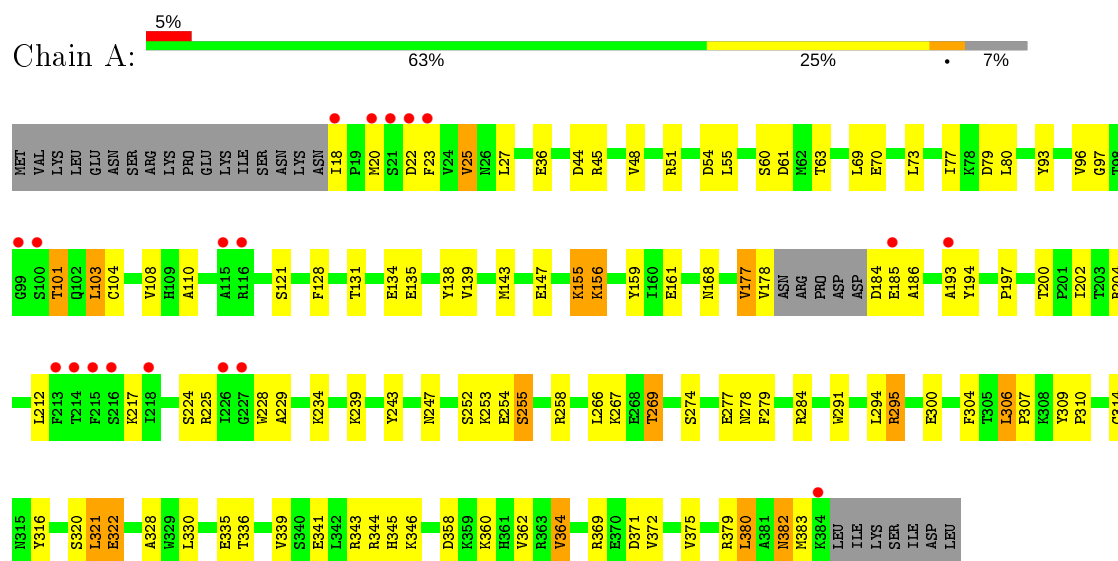
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	102	Total	O	0	0
			102	102		
6	B	129	Total	O	0	0
			129	129		
6	C	90	Total	O	0	0
			90	90		
6	D	100	Total	O	0	0
			100	100		
6	E	75	Total	O	0	0
			75	75		
6	F	96	Total	O	0	0
			96	96		

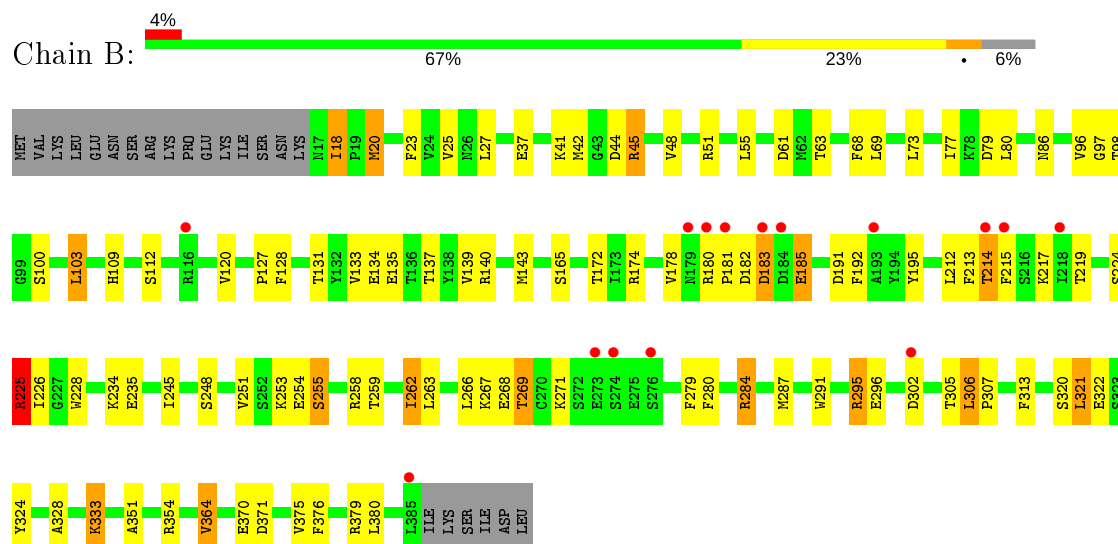
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: L-tryptophan aminotransferase

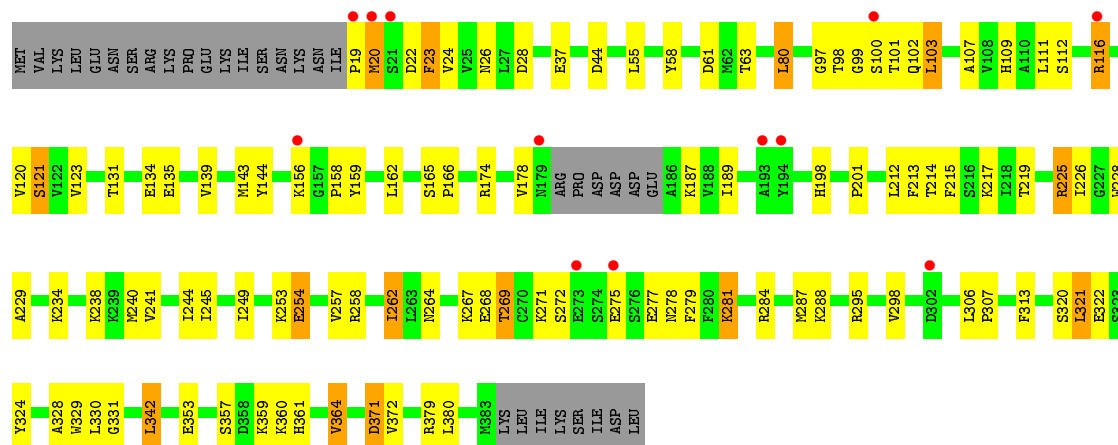


• Molecule 1: L-tryptophan aminotransferase

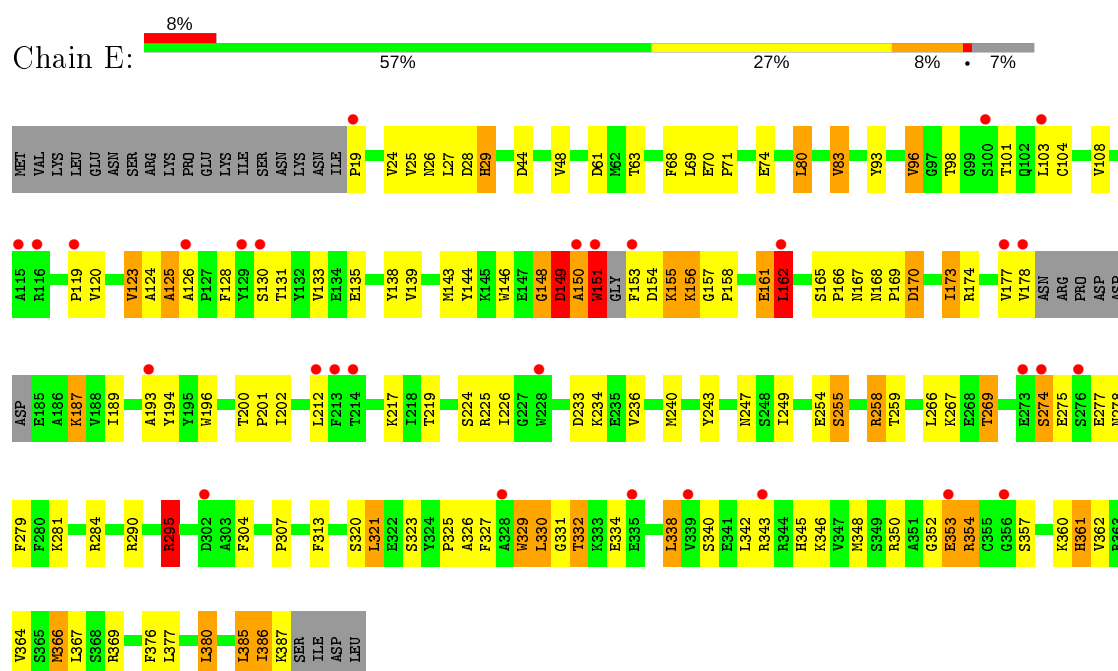


• Molecule 1: L-tryptophan aminotransferase

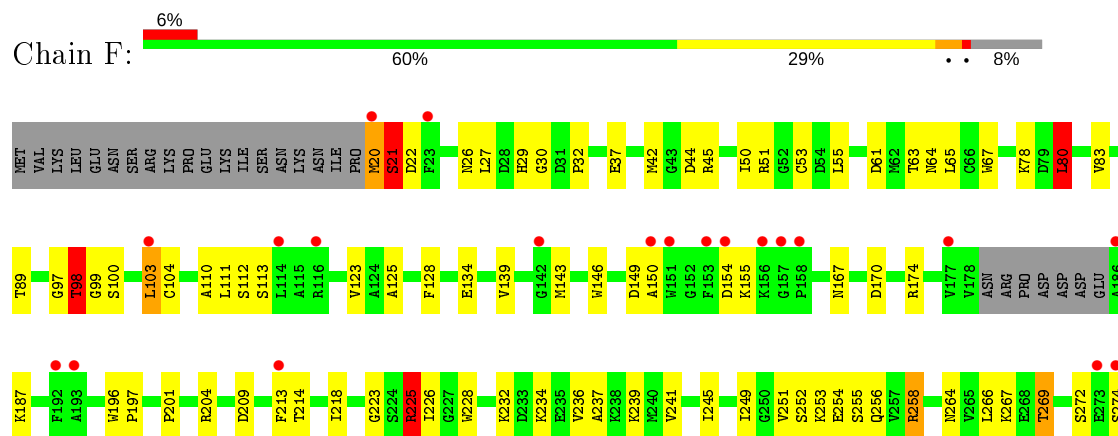


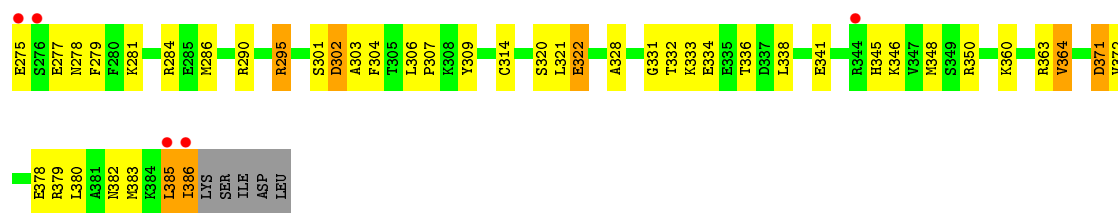


• Molecule 1: L-tryptophan aminotransferase

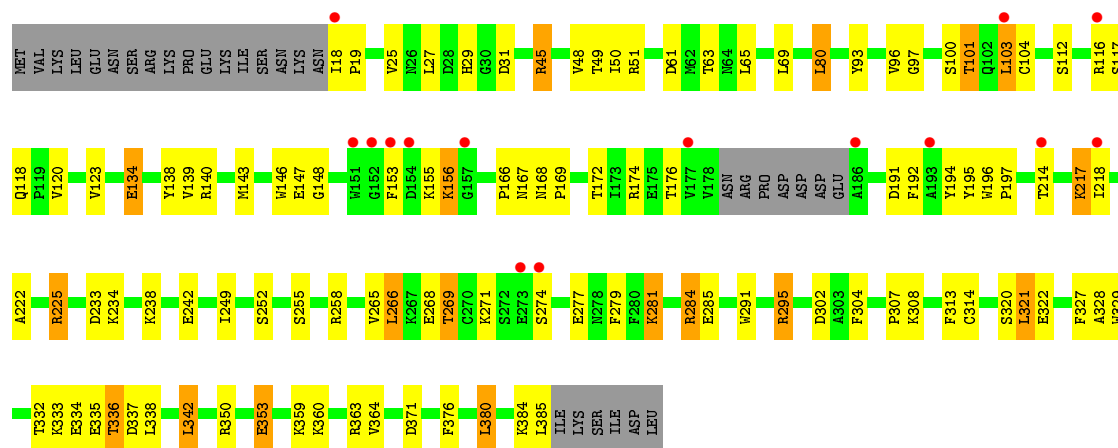


• Molecule 1: L-tryptophan aminotransferase





• Molecule 2: L-tryptophan aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.41 Å 97.83 Å 139.46 Å 90.00° 104.35° 90.00°	Depositor
Resolution (Å)	29.66 – 2.25 29.66 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.66-2.25) 95.9 (29.66-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.56	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.24 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.253 0.222 , 0.239	Depositor DCC
R_{free} test set	5558 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18137	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 31.12 % 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 1.1668e-03. 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, 0.333 respectively for untwinned datasets, and 0.375, 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: PO4, LLP, PMP

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	0.81	1/2975 (0.0%)	0.84	2/4021 (0.0%)
1	B	0.81	0/3033	0.85	4/4104 (0.1%)
1	D	0.83	0/2955	0.88	5/3994 (0.1%)
1	E	0.75	0/2968	0.88	9/4011 (0.2%)
1	F	0.74	0/2960	0.79	3/4000 (0.1%)
2	C	0.79	0/2962	0.83	3/4003 (0.1%)
All	All	0.79	1/17853 (0.0%)	0.85	26/24133 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	E	4	8
1	F	0	1
2	C	0	1
All	All	5	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	ALA	CA-CB	-5.47	1.41	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	225	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	E	321	LEU	CA-CB-CG	8.72	135.36	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	151	TRP	N-CA-C	7.85	132.20	111.00
1	B	321	LEU	CA-CB-CG	7.82	133.29	115.30
1	E	326	ALA	N-CA-C	-7.38	91.06	111.00
2	C	225	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	D	225	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	E	284	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	E	162	LEU	CA-CB-CG	6.13	129.39	115.30
1	A	321	LEU	CA-CB-CG	6.04	129.19	115.30
1	D	80	LEU	CB-CG-CD1	-6.03	100.76	111.00
2	C	342	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	185	GLU	N-CA-C	5.83	126.75	111.00
1	F	80	LEU	CA-CB-CG	5.75	128.54	115.30
1	B	225	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	E	149	ASP	N-CA-C	5.54	125.95	111.00
1	F	225	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	F	258	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	371	ASP	CB-CG-OD2	5.32	123.09	118.30
2	C	191	ASP	CB-CG-OD1	5.32	123.09	118.30
1	E	330	LEU	N-CA-CB	5.32	121.04	110.40
1	E	295	ARG	NE-CZ-NH1	-5.31	117.65	120.30
1	B	225	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	E	155	LYS	CB-CA-C	5.10	120.60	110.40
1	D	342	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	191	ASP	CB-CG-OD2	-5.08	113.73	118.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	185	GLU	CA
1	E	149	ASP	CA
1	E	151	TRP	CA
1	E	155	LYS	CA
1	E	330	LEU	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	217	LLP	Mainchain
1	E	125	ALA	Peptide
1	E	148	GLY	Peptide
1	E	149	ASP	Peptide
1	E	150	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	E	154	ASP	Peptide
1	E	19	PRO	Peptide
1	E	325	PRO	Peptide
1	E	329	TRP	Peptide
1	F	20	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2906	0	2839	83	0
1	B	2962	0	2880	87	0
1	D	2886	0	2810	95	0
1	E	2900	0	2832	131	0
1	F	2892	0	2827	101	0
2	C	2918	0	2847	78	0
3	A	16	0	11	13	0
3	B	16	0	11	8	0
3	D	16	0	4	0	0
3	F	16	0	4	6	0
4	E	5	0	0	1	0
5	F	12	0	0	0	0
6	A	102	0	0	5	0
6	B	129	0	0	6	0
6	C	90	0	0	9	0
6	D	100	0	0	6	0
6	E	75	0	0	5	0
6	F	96	0	0	11	0
All	All	18137	0	17065	565	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 16.

All (565) 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:A:217:LYS:HE3	3:A:1001:PMP:N4A	1.36	1.38
1:B:217:LYS:HE3	3:B:1001:PMP:N4A	1.46	1.25
2:C:218:ILE:HD11	6:C:394:HOH:O	1.35	1.23
1:A:217:LYS:CE	3:A:1001:PMP:HNA2	1.61	1.12
1:B:217:LYS:CE	3:B:1001:PMP:HNA2	1.61	1.12
1:F:67:TRP:CZ2	1:F:245:ILE:HD12	1.94	1.02
1:E:155:LYS:HG3	1:E:156:LYS:H	1.23	1.02
1:E:126:ALA:HB3	1:E:150:ALA:O	1.60	1.01
1:D:98:THR:HG22	1:D:102:GLN:OE1	1.68	0.94
1:E:151:TRP:CZ3	1:E:177:VAL:HG11	2.03	0.94
1:B:217:LYS:HE3	3:B:1001:PMP:HNA2	0.77	0.93
1:E:126:ALA:CB	1:E:150:ALA:O	2.16	0.93
1:E:155:LYS:HG3	1:E:156:LYS:N	1.83	0.91
2:C:217:LLP:C	2:C:218:ILE:HD13	2.01	0.91
1:D:23:PHE:HB2	1:D:379:ARG:HH22	1.39	0.88
1:B:295:ARG:NH2	1:B:307:PRO:O	2.07	0.87
1:E:330:LEU:O	1:E:361:HIS:HA	1.74	0.87
2:C:266:LEU:O	2:C:269:THR:HG22	1.75	0.86
1:F:20:MET:O	1:F:21:SER:HB3	1.74	0.86
1:D:61:ASP:OD1	1:D:63:THR:HB	1.76	0.85
1:A:252:SER:HB3	1:A:255:SER:HB2	1.57	0.85
1:A:217:LYS:HE3	3:A:1001:PMP:HNA2	0.71	0.84
1:A:101:THR:HG22	3:A:1001:PMP:O2P	1.78	0.83
3:A:1001:PMP:N4A	3:A:1001:PMP:H5A2	1.93	0.82
1:B:266:LEU:O	1:B:269:THR:HG22	1.79	0.82
1:D:284:ARG:NH2	1:D:322:GLU:O	2.13	0.81
1:E:167:ASN:HD22	1:E:170:ASP:HB2	1.45	0.81
1:A:217:LYS:CE	3:A:1001:PMP:N4A	2.28	0.81
1:E:354:ARG:CG	1:E:354:ARG:HH11	1.92	0.81
1:E:274:SER:HB3	1:E:277:GLU:HB2	1.63	0.81
1:A:61:ASP:OD1	1:A:63:THR:HB	1.81	0.80
1:E:74:GLU:OE1	6:E:1021:HOH:O	1.99	0.79
1:E:151:TRP:CE3	1:E:177:VAL:HG11	2.17	0.79
2:C:284:ARG:NH2	2:C:322:GLU:O	2.15	0.79
1:A:22:ASP:HA	1:A:346:LYS:HD2	1.64	0.79
1:A:44:ASP:OD1	1:B:51:ARG:NH2	2.17	0.78
1:E:155:LYS:CG	1:E:156:LYS:H	1.96	0.78
1:F:64:ASN:HB3	6:F:2018:HOH:O	1.83	0.77
2:C:45:ARG:HD2	2:C:265:VAL:HG13	1.64	0.77
2:C:281:LYS:HE2	6:C:395:HOH:O	1.83	0.76
1:E:334:GLU:HG2	1:E:387:LYS:HG2	1.68	0.76
2:C:214:THR:O	2:C:218:ILE:HG12	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:ILE:HD13	6:F:2064:HOH:O	1.86	0.75
1:D:201:PRO:HG3	1:D:321:LEU:HD23	1.69	0.74
2:C:338:LEU:O	2:C:342:LEU:HD22	1.86	0.74
1:D:159:TYR:OH	1:D:178:VAL:HG11	1.87	0.74
1:A:69:LEU:HD13	1:A:96:VAL:HG13	1.69	0.74
1:F:104:CYS:HB2	6:F:2054:HOH:O	1.86	0.74
1:D:19:PRO:O	1:D:23:PHE:CZ	2.40	0.74
1:A:60:SER:OG	1:A:70:GLU:OE2	2.05	0.74
1:B:18:ILE:H	1:B:18:ILE:HD13	1.53	0.73
1:F:225:ARG:NE	1:F:225:ARG:HA	2.04	0.72
3:A:1001:PMP:HNA1	3:A:1001:PMP:H5A2	1.54	0.72
1:E:153:PHE:CE1	1:E:155:LYS:HB3	2.24	0.72
2:C:295:ARG:NH2	2:C:307:PRO:O	2.23	0.72
2:C:104:CYS:HB2	6:C:471:HOH:O	1.88	0.72
2:C:197:PRO:O	2:C:284:ARG:NH1	2.21	0.72
1:F:149:ASP:OD1	1:F:150:ALA:N	2.22	0.72
1:F:341:GLU:O	1:F:345:HIS:HD2	1.74	0.71
1:E:150:ALA:O	1:E:151:TRP:HD1	1.74	0.71
2:C:274:SER:HB3	2:C:277:GLU:HB2	1.73	0.70
1:E:126:ALA:HB3	1:E:150:ALA:C	2.12	0.70
1:B:225:ARG:HH22	3:B:1001:PMP:P	2.14	0.70
2:C:112:SER:HA	2:C:120:VAL:HG21	1.73	0.70
1:E:330:LEU:O	1:E:361:HIS:CA	2.39	0.70
1:E:354:ARG:HA	6:E:1075:HOH:O	1.90	0.70
1:E:27:LEU:HB3	1:E:364:VAL:HG13	1.72	0.70
1:F:97:GLY:HA2	1:F:251:VAL:HG21	1.72	0.70
3:A:1001:PMP:C5A	3:A:1001:PMP:HNA1	2.04	0.69
1:E:354:ARG:HH11	1:E:354:ARG:HG3	1.57	0.69
1:A:202:ILE:HD13	1:A:316:TYR:CB	2.23	0.69
1:E:120:VAL:H	1:E:144:TYR:HA	1.57	0.69
1:E:125:ALA:O	1:E:174:ARG:NH1	2.26	0.68
1:E:125:ALA:HA	1:E:126:ALA:HB3	1.74	0.68
1:E:274:SER:CB	1:E:277:GLU:HB2	2.23	0.68
1:E:151:TRP:CZ3	1:E:177:VAL:CG1	2.76	0.68
2:C:93:TYR:OH	2:C:234:LYS:HE2	1.94	0.68
1:E:151:TRP:CZ2	1:E:177:VAL:HG21	2.29	0.67
1:E:352:GLY:O	1:E:354:ARG:N	2.27	0.67
2:C:238:LYS:O	2:C:242:GLU:HG3	1.95	0.66
1:A:36:GLU:CD	1:A:369:ARG:HH12	1.99	0.66
1:D:20:MET:HA	1:D:23:PHE:CZ	2.31	0.66
1:E:161:GLU:O	1:E:162:LEU:HD23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:THR:HG23	1:E:278:ASN:HA	1.78	0.66
1:E:123:VAL:HA	1:E:148:GLY:O	1.96	0.65
1:F:269:THR:O	1:F:272:SER:HB3	1.96	0.65
1:A:274:SER:HB3	1:A:277:GLU:HB2	1.79	0.65
1:E:151:TRP:CH2	1:E:177:VAL:HG11	2.32	0.65
1:A:156:LYS:H	1:A:156:LYS:HD2	1.62	0.65
1:D:116:ARG:H	1:D:116:ARG:HE	1.45	0.65
1:A:346:LYS:HB2	1:A:379:ARG:NH1	2.13	0.64
1:E:151:TRP:CD1	1:E:151:TRP:N	2.64	0.64
1:F:385:LEU:HD23	1:F:386:ILE:HG22	1.80	0.64
1:F:197:PRO:O	1:F:284:ARG:NH1	2.32	0.63
1:E:126:ALA:HB1	1:E:150:ALA:O	1.98	0.63
1:E:123:VAL:HG12	1:E:148:GLY:H	1.63	0.63
1:E:224:SER:O	1:E:255:SER:OG	2.17	0.63
1:A:266:LEU:O	1:A:269:THR:HG22	1.99	0.63
1:E:44:ASP:OD1	1:F:51:ARG:NH2	2.31	0.63
1:F:241:VAL:O	1:F:245:ILE:HG12	1.98	0.63
1:D:307:PRO:HD3	1:D:329:TRP:O	1.99	0.62
3:A:1001:PMP:N4A	3:A:1001:PMP:C5A	2.60	0.62
1:D:139:VAL:HG22	6:D:1009:HOH:O	1.99	0.62
2:C:269:THR:HG23	2:C:279:PHE:H	1.64	0.62
1:D:23:PHE:HB2	1:D:379:ARG:NH2	2.12	0.62
1:E:61:ASP:OD2	1:E:63:THR:HB	2.00	0.62
1:F:98:THR:O	1:F:98:THR:OG1	2.14	0.62
1:E:104:CYS:O	1:E:108:VAL:HG23	1.99	0.62
1:E:124:ALA:O	1:E:128:PHE:HD2	1.82	0.62
1:D:225:ARG:HA	1:D:225:ARG:NE	2.15	0.62
1:D:107:ALA:HB2	1:D:240:MET:CE	2.29	0.62
1:F:110:ALA:HB1	1:F:239:LYS:HB2	1.81	0.62
2:C:80:LEU:HD21	2:C:266:LEU:HD21	1.82	0.62
1:B:61:ASP:OD1	1:B:63:THR:HB	1.98	0.61
1:D:241:VAL:O	1:D:245:ILE:HG12	2.00	0.61
1:F:269:THR:CG2	1:F:279:PHE:H	2.13	0.61
1:A:143:MET:HG2	1:B:140:ARG:HD3	1.81	0.61
1:D:215:PHE:HZ	1:D:262:ILE:HG12	1.65	0.61
1:E:173:ILE:N	1:E:173:ILE:HD13	2.15	0.61
2:C:97:GLY:HA3	2:C:103:LEU:HD13	1.81	0.61
1:A:143:MET:CG	1:B:140:ARG:HD3	2.31	0.61
1:E:330:LEU:O	1:E:361:HIS:HB3	2.00	0.61
1:E:165:SER:HA	1:E:166:PRO:C	2.20	0.61
1:E:130:SER:HB2	1:E:354:ARG:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:CYS:SG	6:F:2086:HOH:O	2.56	0.60
2:C:61:ASP:OD1	2:C:63:THR:HB	2.01	0.60
1:B:219:THR:HG21	1:B:262:ILE:HD11	1.82	0.60
1:B:215:PHE:HZ	1:B:262:ILE:HG12	1.65	0.60
1:F:167:ASN:HB3	1:F:170:ASP:OD1	2.02	0.60
1:A:202:ILE:HD13	1:A:316:TYR:HB2	1.84	0.59
1:A:25:VAL:HG22	1:A:372:VAL:HG13	1.84	0.59
1:B:73:LEU:O	1:B:77:ILE:HG12	2.02	0.59
1:E:128:PHE:O	1:E:169:PRO:HD3	2.02	0.59
1:A:202:ILE:HD13	1:A:316:TYR:HB3	1.83	0.59
1:A:224:SER:HA	1:B:254:GLU:OE1	2.02	0.59
1:E:162:LEU:HA	1:E:189:ILE:O	2.02	0.59
1:B:79:ASP:HB3	1:B:267:LYS:HE2	1.84	0.59
1:A:284:ARG:NH2	1:A:322:GLU:O	2.36	0.59
2:C:18:ILE:HG13	2:C:19:PRO:HD3	1.85	0.59
1:B:217:LYS:CE	3:B:1001:PMP:N4A	2.38	0.59
1:D:103:LEU:HD21	1:D:228:TRP:HA	1.85	0.59
1:D:287:MET:HB3	1:D:324:TYR:HB3	1.85	0.59
2:C:268:GLU:O	2:C:271:LYS:HG2	2.03	0.59
1:E:28:ASP:OD1	1:E:350:ARG:HD2	2.03	0.59
1:D:295:ARG:NH2	1:D:307:PRO:O	2.35	0.58
1:E:126:ALA:CB	1:E:150:ALA:C	2.70	0.58
1:F:322:GLU:HB3	6:F:2039:HOH:O	2.03	0.58
2:C:269:THR:CG2	2:C:279:PHE:H	2.16	0.58
2:C:376:PHE:O	2:C:380:LEU:HB2	2.03	0.58
1:A:266:LEU:HD13	1:A:279:PHE:HB3	1.86	0.58
2:C:48:VAL:HG21	2:C:258:ARG:HG3	1.85	0.58
1:D:26:ASN:OD1	1:D:28:ASP:HB3	2.03	0.58
1:A:375:VAL:O	1:A:379:ARG:HG3	2.04	0.58
1:E:48:VAL:HG21	1:E:258:ARG:HD2	1.86	0.58
1:D:131:THR:O	1:D:135:GLU:HG3	2.04	0.57
1:E:354:ARG:HG2	1:E:354:ARG:HH11	1.69	0.57
1:F:26:ASN:HA	1:F:348:MET:HB2	1.84	0.57
1:D:328:ALA:HB3	1:D:364:VAL:HG22	1.85	0.57
1:E:177:VAL:HG12	1:E:177:VAL:O	2.03	0.57
1:E:354:ARG:NH1	1:E:354:ARG:HG3	2.15	0.57
1:E:332:THR:O	1:E:360:LYS:HD3	2.04	0.57
1:A:69:LEU:HD13	1:A:96:VAL:CG1	2.34	0.57
1:E:193:ALA:HB2	6:E:1068:HOH:O	2.04	0.57
1:B:27:LEU:HB3	1:B:364:VAL:HG23	1.85	0.57
1:E:123:VAL:CA	1:E:148:GLY:O	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:SER:OG	1:F:143:MET:HB3	2.04	0.57
1:F:65:LEU:HD23	1:F:241:VAL:HG21	1.86	0.57
1:A:339:VAL:O	1:A:343:ARG:HG3	2.05	0.57
1:E:68:PHE:HE2	1:E:96:VAL:HG23	1.70	0.57
1:B:20:MET:HE2	1:B:23:PHE:HB2	1.87	0.57
1:E:354:ARG:CG	1:E:354:ARG:NH1	2.60	0.57
1:B:328:ALA:HB3	1:B:364:VAL:HG13	1.86	0.56
1:B:98:THR:O	1:B:98:THR:OG1	2.14	0.56
1:E:226:ILE:HD11	1:E:255:SER:HB3	1.87	0.56
2:C:29:HIS:ND1	2:C:31:ASP:HB2	2.19	0.56
1:D:107:ALA:HB2	1:D:240:MET:HE1	1.87	0.56
1:F:214:THR:O	1:F:214:THR:HG23	2.04	0.56
1:D:19:PRO:O	1:D:23:PHE:CE2	2.58	0.56
1:D:268:GLU:O	1:D:271:LYS:HG2	2.05	0.56
1:E:125:ALA:HB1	1:E:151:TRP:HE1	1.69	0.56
1:E:83:VAL:HG11	1:E:267:LYS:HG3	1.88	0.56
2:C:45:ARG:HD2	2:C:265:VAL:CG1	2.33	0.56
1:E:385:LEU:O	1:E:386:ILE:HB	2.05	0.56
1:A:104:CYS:HB2	6:A:1078:HOH:O	2.06	0.56
1:D:240:MET:O	1:D:244:ILE:HG12	2.04	0.56
1:F:209:ASP:HA	1:F:232:LYS:HD2	1.88	0.56
1:D:264:ASN:O	1:D:268:GLU:HG3	2.05	0.56
1:B:97:GLY:HA3	1:B:103:LEU:HD13	1.87	0.56
1:B:291:TRP:O	1:B:295:ARG:HB2	2.05	0.55
1:F:97:GLY:C	6:F:2064:HOH:O	2.44	0.55
1:A:177:VAL:HG23	1:A:177:VAL:O	2.06	0.55
1:A:328:ALA:HB3	1:A:364:VAL:HG13	1.88	0.55
1:D:100:SER:HB2	6:D:1046:HOH:O	2.05	0.55
1:E:226:ILE:HD13	1:E:259:THR:OG1	2.04	0.55
1:A:266:LEU:HD12	1:A:266:LEU:O	2.06	0.55
2:C:169:PRO:HB2	2:C:329:TRP:CE3	2.42	0.55
1:E:334:GLU:CG	1:E:387:LYS:HG2	2.37	0.55
1:A:168:ASN:ND2	3:A:1001:PMP:O3	2.38	0.55
1:F:22:ASP:HA	1:F:346:LYS:NZ	2.21	0.55
1:D:120:VAL:H	1:D:144:TYR:HA	1.72	0.55
1:E:342:LEU:O	1:E:345:HIS:N	2.37	0.55
1:A:73:LEU:O	1:A:77:ILE:HG12	2.07	0.55
1:F:303:ALA:O	1:F:332:THR:HA	2.07	0.55
1:F:201:PRO:HB3	1:F:314:CYS:HB2	1.89	0.55
1:B:112:SER:HA	1:B:120:VAL:HG21	1.89	0.54
1:D:159:TYR:OH	1:D:178:VAL:CG1	2.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:THR:HA	1:F:225:ARG:O	2.06	0.54
1:A:104:CYS:O	1:A:108:VAL:HG23	2.07	0.54
1:A:382:ASN:N	1:A:382:ASN:HD22	2.05	0.54
1:F:269:THR:HG23	1:F:278:ASN:HA	1.88	0.54
1:B:55:LEU:HB3	1:B:253:LYS:HB3	1.90	0.54
1:D:98:THR:HA	1:D:225:ARG:O	2.07	0.54
1:E:131:THR:O	1:E:135:GLU:HG3	2.08	0.54
1:F:382:ASN:O	1:F:385:LEU:HB3	2.08	0.54
1:B:98:THR:HG22	6:B:1015:HOH:O	2.06	0.54
1:F:42:MET:HE3	1:F:45:ARG:HD3	1.88	0.54
1:A:194:TYR:HE2	3:A:1001:PMP:HO3	1.53	0.54
1:D:269:THR:CG2	1:D:279:PHE:H	2.21	0.54
1:B:284:ARG:NH2	1:B:322:GLU:O	2.35	0.54
1:E:148:GLY:HA3	1:E:149:ASP:O	2.08	0.54
1:E:139:VAL:HG11	1:F:139:VAL:HB	1.90	0.54
1:A:346:LYS:HB2	1:A:379:ARG:HH12	1.73	0.54
1:B:133:VAL:O	1:B:137:THR:HB	2.08	0.53
1:A:51:ARG:NH2	1:B:44:ASP:CG	2.61	0.53
1:B:215:PHE:HZ	1:B:262:ILE:CG1	2.20	0.53
1:B:295:ARG:HD3	6:B:1034:HOH:O	2.08	0.53
1:D:269:THR:HG23	1:D:278:ASN:HA	1.89	0.53
1:B:100:SER:N	3:B:1001:PMP:O2P	2.41	0.53
1:B:225:ARG:HA	1:B:225:ARG:NE	2.23	0.53
2:C:167:ASN:HB2	2:C:174:ARG:HD2	1.91	0.53
1:B:98:THR:HA	1:B:225:ARG:O	2.09	0.53
2:C:337:ASP:HA	2:C:359:LYS:HB3	1.91	0.53
2:C:140:ARG:HD3	1:D:143:MET:HG2	1.91	0.53
1:E:330:LEU:O	1:E:361:HIS:CB	2.56	0.53
1:E:80:LEU:HD21	1:E:266:LEU:HD23	1.90	0.53
1:A:341:GLU:OE1	1:A:344:ARG:NH1	2.42	0.53
1:E:269:THR:CG2	1:E:279:PHE:H	2.21	0.53
1:B:181:PRO:C	1:B:183:ASP:N	2.61	0.53
1:F:284:ARG:NH2	1:F:322:GLU:O	2.42	0.53
1:A:330:LEU:HB3	1:A:362:VAL:HG23	1.91	0.52
2:C:214:THR:O	2:C:218:ILE:CG1	2.56	0.52
1:D:272:SER:HB2	6:D:1070:HOH:O	2.08	0.52
1:A:291:TRP:O	1:A:295:ARG:HB2	2.09	0.52
1:B:268:GLU:O	1:B:271:LYS:HG2	2.09	0.52
2:C:302:ASP:O	2:C:333:LYS:HD2	2.08	0.52
1:A:330:LEU:HB3	1:A:362:VAL:CG2	2.39	0.52
2:C:350:ARG:HB3	2:C:363:ARG:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:LEU:HB3	1:E:362:VAL:HG13	1.91	0.52
1:E:330:LEU:HA	1:E:362:VAL:O	2.08	0.52
1:E:101:THR:HG22	4:E:1001:PO4:O3	2.09	0.52
1:F:226:ILE:HA	6:F:2064:HOH:O	2.10	0.52
1:B:18:ILE:H	1:B:18:ILE:CD1	2.22	0.52
1:D:116:ARG:NE	1:D:116:ARG:H	2.08	0.52
1:D:219:THR:HG21	1:D:262:ILE:HD11	1.92	0.52
1:F:125:ALA:O	1:F:174:ARG:NH1	2.43	0.52
2:C:100:SER:N	2:C:217:LLP:OP2	2.42	0.52
1:E:219:THR:HG22	1:E:266:LEU:HD13	1.92	0.52
1:E:313:PHE:HA	1:E:320:SER:HA	1.92	0.52
1:A:51:ARG:HH21	1:B:44:ASP:CG	2.13	0.52
1:E:74:GLU:CG	6:E:1021:HOH:O	2.58	0.51
1:F:304:PHE:HE1	1:F:338:LEU:HD11	1.74	0.51
2:C:196:TRP:CD1	2:C:218:ILE:HD12	2.45	0.51
1:E:126:ALA:CB	1:E:150:ALA:HA	2.40	0.51
1:E:338:LEU:CD1	1:E:342:LEU:HD13	2.40	0.51
1:F:284:ARG:NE	6:F:2027:HOH:O	2.36	0.51
1:F:303:ALA:HA	1:F:333:LYS:HD2	1.92	0.51
1:B:180:ARG:HD3	6:B:1025:HOH:O	2.10	0.51
1:D:97:GLY:HA3	1:D:103:LEU:HD13	1.93	0.51
1:E:367:LEU:HD12	6:E:1065:HOH:O	2.11	0.51
1:B:77:ILE:HD12	1:B:228:TRP:CD2	2.46	0.50
1:E:124:ALA:N	1:E:148:GLY:O	2.42	0.50
1:A:224:SER:O	1:A:255:SER:OG	2.30	0.50
1:B:42:MET:O	1:B:45:ARG:HG2	2.11	0.50
1:D:298:VAL:HG21	1:D:306:LEU:HD22	1.94	0.50
1:D:234:LYS:O	1:D:238:LYS:HB2	2.11	0.50
1:E:236:VAL:O	1:E:240:MET:HG3	2.11	0.50
2:C:314:CYS:HB2	2:C:321:LEU:HD11	1.93	0.50
2:C:168:ASN:ND2	2:C:327:PHE:CE2	2.80	0.50
1:F:22:ASP:OD2	1:F:346:LYS:NZ	2.44	0.50
2:C:304:PHE:CE2	2:C:380:LEU:HD22	2.47	0.49
1:B:226:ILE:HG21	1:B:259:THR:HG21	1.95	0.49
1:B:259:THR:O	1:B:263:LEU:HG	2.12	0.49
1:B:296:GLU:HB2	6:B:1033:HOH:O	2.11	0.49
1:E:120:VAL:HG22	1:E:158:PRO:HB2	1.93	0.49
1:F:97:GLY:HA2	1:F:251:VAL:CG2	2.41	0.49
1:B:131:THR:O	1:B:135:GLU:HG3	2.12	0.49
1:B:183:ASP:C	1:B:185:GLU:H	2.16	0.49
1:A:371:ASP:O	1:A:375:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ASN:HB2	1:B:195:TYR:CD2	2.46	0.49
2:C:69:LEU:HD13	2:C:96:VAL:HB	1.94	0.49
1:E:119:PRO:HA	1:E:143:MET:O	2.12	0.49
1:B:45:ARG:NH2	1:B:268:GLU:OE2	2.46	0.49
1:B:217:LYS:HG3	3:B:1001:PMP:HNA1	1.77	0.49
2:C:238:LYS:HE3	2:C:242:GLU:OE2	2.12	0.49
1:F:281:LYS:HD3	1:F:281:LYS:C	2.33	0.49
1:A:23:PHE:HB3	1:A:379:ARG:HH22	1.78	0.49
1:B:139:VAL:HG22	6:B:1010:HOH:O	2.12	0.49
1:F:67:TRP:HZ2	1:F:245:ILE:HD12	1.66	0.49
2:C:225:ARG:NH1	2:C:225:ARG:HA	2.28	0.49
1:E:254:GLU:OE2	1:F:258:ARG:HD3	2.13	0.49
1:F:225:ARG:CZ	1:F:225:ARG:HA	2.43	0.49
1:E:161:GLU:O	1:E:162:LEU:CD2	2.61	0.48
1:F:274:SER:HB3	1:F:277:GLU:HB2	1.94	0.48
1:F:309:TYR:HB2	6:F:2039:HOH:O	2.14	0.48
1:D:198:HIS:HA	1:D:284:ARG:HB2	1.95	0.48
1:D:23:PHE:N	1:D:23:PHE:CD2	2.80	0.48
1:E:290:ARG:NH1	1:E:366:MET:O	2.44	0.48
1:E:68:PHE:CE2	1:E:96:VAL:HG23	2.49	0.48
1:F:379:ARG:O	1:F:383:MET:HB2	2.14	0.48
1:F:61:ASP:OD2	1:F:63:THR:HB	2.13	0.48
2:C:49:THR:O	2:C:50:ILE:HD13	2.14	0.48
1:E:194:TYR:OH	1:E:217:LYS:NZ	2.41	0.48
1:B:181:PRO:O	1:B:183:ASP:N	2.47	0.48
1:E:274:SER:HB3	1:E:277:GLU:H	1.79	0.48
1:E:93:TYR:CE2	1:E:234:LYS:HA	2.49	0.48
1:B:375:VAL:O	1:B:379:ARG:HG3	2.14	0.48
1:D:19:PRO:HG3	1:D:22:ASP:OD1	2.14	0.48
1:E:27:LEU:CB	1:E:364:VAL:HG13	2.40	0.48
1:F:167:ASN:HB2	1:F:174:ARG:HD2	1.95	0.48
1:B:172:THR:HG22	1:B:174:ARG:HG2	1.95	0.47
2:C:218:ILE:N	2:C:218:ILE:HD13	2.29	0.47
1:E:98:THR:HA	1:E:225:ARG:O	2.13	0.47
1:E:26:ASN:HA	1:E:348:MET:HB2	1.96	0.47
2:C:65:LEU:HD11	2:C:238:LYS:HB2	1.96	0.47
2:C:194:TYR:CE1	2:C:217:LLP:HB2	2.49	0.47
2:C:313:PHE:HB3	6:C:478:HOH:O	2.13	0.47
2:C:291:TRP:O	2:C:295:ARG:HB2	2.14	0.47
1:D:120:VAL:N	1:D:144:TYR:HA	2.30	0.47
1:D:159:TYR:CZ	1:D:178:VAL:HG11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:GLY:C	1:E:354:ARG:H	2.17	0.47
2:C:123:VAL:HG12	2:C:147:GLU:HB2	1.96	0.47
1:D:330:LEU:O	1:D:361:HIS:HA	2.15	0.47
1:A:295:ARG:NH2	1:A:307:PRO:O	2.47	0.47
1:E:69:LEU:HD21	1:E:74:GLU:HG3	1.97	0.47
1:B:262:ILE:HD12	1:B:262:ILE:C	2.35	0.46
2:C:80:LEU:HD13	2:C:196:TRP:CH2	2.49	0.46
1:E:151:TRP:N	1:E:151:TRP:HD1	2.12	0.46
2:C:139:VAL:HA	1:D:143:MET:HE1	1.97	0.46
1:F:111:LEU:HD22	1:F:187:LYS:HE3	1.98	0.46
1:F:334:GLU:HB3	1:F:336:THR:HG23	1.96	0.46
1:B:269:THR:CG2	1:B:279:PHE:H	2.28	0.46
1:F:252:SER:O	1:F:256:GLN:HG3	2.16	0.46
1:F:253:LYS:HE2	6:F:2041:HOH:O	2.14	0.46
1:B:48:VAL:HG21	1:B:258:ARG:HG3	1.97	0.46
1:B:69:LEU:HD13	1:B:96:VAL:HB	1.97	0.46
2:C:176:THR:HG23	6:C:408:HOH:O	2.16	0.46
2:C:335:GLU:HG3	2:C:360:LYS:HE3	1.98	0.46
1:A:225:ARG:HH22	3:A:1001:PMP:P	2.38	0.46
1:B:68:PHE:CE1	1:B:245:ILE:CD1	2.99	0.46
2:C:134:GLU:HG2	2:C:134:GLU:H	1.28	0.46
1:D:23:PHE:HD2	1:D:23:PHE:N	2.14	0.46
1:D:288:LYS:HG3	1:D:324:TYR:CZ	2.50	0.46
1:D:353:GLU:OE1	1:D:359:LYS:HG3	2.16	0.46
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.75	0.46
1:D:275:GLU:HG2	1:D:281:LYS:HD2	1.97	0.46
1:F:196:TRP:HB3	1:F:197:PRO:HD2	1.98	0.46
1:B:219:THR:HG22	1:B:266:LEU:HD12	1.98	0.46
1:D:102:GLN:HG2	1:D:244:ILE:CD1	2.46	0.46
1:A:200:THR:HB	6:A:1095:HOH:O	2.16	0.46
1:A:139:VAL:HA	1:B:143:MET:HE1	1.98	0.46
1:D:213:PHE:C	6:D:1046:HOH:O	2.54	0.46
1:E:80:LEU:HD13	1:E:196:TRP:CH2	2.51	0.46
1:D:23:PHE:O	1:D:379:ARG:NH1	2.49	0.45
1:F:111:LEU:HD22	1:F:187:LYS:HG2	1.98	0.45
1:F:371:ASP:OD2	1:F:372:VAL:HG23	2.16	0.45
1:A:55:LEU:HB3	1:A:253:LYS:HB3	1.99	0.45
1:A:93:TYR:N	1:A:93:TYR:CD2	2.84	0.45
1:B:25:VAL:HG11	1:B:376:PHE:HB2	1.99	0.45
1:E:165:SER:HA	1:E:167:ASN:N	2.30	0.45
1:E:25:VAL:HG11	1:E:376:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:101:THR:HG22	2:C:217:LLP:H5'2	1.98	0.45
1:E:161:GLU:HG3	1:E:178:VAL:CG1	2.47	0.45
1:E:269:THR:HG21	1:E:279:PHE:H	1.80	0.45
1:B:172:THR:HG23	6:B:1114:HOH:O	2.16	0.45
1:D:131:THR:HG22	1:D:135:GLU:HG3	1.99	0.45
1:E:295:ARG:NH2	1:E:307:PRO:O	2.49	0.45
1:A:193:ALA:HB2	6:A:1039:HOH:O	2.17	0.45
1:D:162:LEU:HD23	1:D:189:ILE:HB	1.98	0.45
1:B:280:PHE:O	1:B:284:ARG:HB2	2.17	0.45
1:D:55:LEU:HB3	1:D:253:LYS:HB3	1.97	0.45
1:F:303:ALA:HB1	1:F:333:LYS:HB2	1.97	0.45
1:F:27:LEU:HD13	1:F:364:VAL:HG23	1.99	0.45
1:F:37:GLU:HB3	6:F:2070:HOH:O	2.17	0.45
2:C:27:LEU:HA	6:C:466:HOH:O	2.17	0.45
2:C:332:THR:HG23	2:C:334:GLU:O	2.17	0.45
2:C:45:ARG:HB3	6:C:436:HOH:O	2.17	0.45
1:D:331:GLY:HA2	1:D:360:LYS:O	2.17	0.45
1:E:155:LYS:CG	1:E:156:LYS:N	2.61	0.45
1:D:201:PRO:HG3	1:D:321:LEU:CD2	2.45	0.45
1:A:304:PHE:CE2	1:A:380:LEU:HD22	2.52	0.44
1:D:287:MET:HB3	1:D:324:TYR:CB	2.48	0.44
1:F:266:LEU:O	1:F:269:THR:HB	2.17	0.44
1:F:55:LEU:HD13	1:F:253:LYS:HB3	1.98	0.44
1:A:159:TYR:CE1	1:A:186:ALA:CB	3.00	0.44
1:D:111:LEU:HD22	1:D:187:LYS:HG3	1.99	0.44
1:F:111:LEU:HD22	1:F:187:LYS:CG	2.47	0.44
1:A:156:LYS:CD	1:A:156:LYS:H	2.29	0.44
2:C:166:PRO:HA	2:C:172:THR:O	2.17	0.44
2:C:249:ILE:HG13	1:D:101:THR:HG21	1.99	0.44
1:E:123:VAL:O	1:E:161:GLU:O	2.35	0.44
1:E:243:TYR:O	1:E:247:ASN:HB2	2.17	0.44
1:F:213:PHE:HB2	1:F:228:TRP:NE1	2.32	0.44
1:F:80:LEU:HA	1:F:83:VAL:HG12	1.99	0.44
1:A:269:THR:CG2	1:A:279:PHE:H	2.31	0.44
1:A:291:TRP:HH2	6:A:1092:HOH:O	2.00	0.44
2:C:222:ALA:HB1	1:D:58:TYR:CZ	2.53	0.44
1:A:225:ARG:HA	1:A:225:ARG:CZ	2.47	0.44
1:A:345:HIS:CE1	1:A:383:MET:HB3	2.53	0.44
2:C:328:ALA:HB3	2:C:364:VAL:HG13	1.99	0.44
1:E:173:ILE:HD12	1:E:173:ILE:HA	1.77	0.44
1:E:377:LEU:O	1:E:380:LEU:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:THR:CG2	1:F:214:THR:O	2.65	0.44
1:F:249:ILE:O	1:F:249:ILE:HG22	2.18	0.44
1:A:155:LYS:HA	1:A:156:LYS:HE2	1.99	0.44
1:B:305:THR:HG22	1:B:333:LYS:HE2	2.00	0.44
2:C:139:VAL:HG22	6:C:430:HOH:O	2.17	0.44
1:F:123:VAL:HG23	1:F:150:ALA:HB2	1.99	0.44
2:C:308:LYS:HB3	2:C:308:LYS:HE2	1.78	0.44
1:E:29:HIS:O	1:E:29:HIS:ND1	2.46	0.44
1:A:79:ASP:HB3	1:A:267:LYS:CD	2.47	0.44
2:C:51:ARG:NH2	1:D:44:ASP:OD2	2.50	0.44
1:F:295:ARG:NH2	1:F:307:PRO:O	2.50	0.44
1:A:97:GLY:HA3	1:A:103:LEU:HD13	1.99	0.44
1:D:121:SER:O	1:D:159:TYR:HA	2.18	0.44
1:E:150:ALA:C	1:E:151:TRP:HD1	2.20	0.44
1:E:133:VAL:HG22	1:E:146:TRP:CZ2	2.53	0.43
1:F:225:ARG:NE	1:F:225:ARG:CA	2.76	0.43
2:C:118:GLN:HB3	2:C:143:MET:HA	2.00	0.43
1:E:148:GLY:CA	1:E:149:ASP:O	2.66	0.43
1:E:226:ILE:HD11	1:E:255:SER:CB	2.47	0.43
1:F:22:ASP:HA	1:F:346:LYS:HZ3	1.82	0.43
1:B:68:PHE:CE1	1:B:245:ILE:HD11	2.54	0.43
1:D:111:LEU:HD12	1:D:189:ILE:HD11	2.00	0.43
1:F:30:GLY:O	1:F:32:PRO:HD3	2.18	0.43
1:E:70:GLU:HA	1:E:71:PRO:HD2	1.87	0.43
1:F:29:HIS:ND1	1:F:29:HIS:O	2.52	0.43
1:A:103:LEU:HD21	1:A:228:TRP:HA	2.01	0.43
1:B:215:PHE:CZ	1:B:262:ILE:CG1	3.01	0.43
1:A:204:ARG:HH22	1:F:204:ARG:HD3	1.84	0.43
1:D:165:SER:HB2	1:D:174:ARG:HB2	2.00	0.43
1:D:275:GLU:CG	1:D:281:LYS:HD2	2.49	0.43
1:A:161:GLU:OE2	1:A:178:VAL:HG12	2.19	0.43
1:A:197:PRO:HB3	1:A:202:ILE:HD11	2.00	0.43
2:C:336:THR:HG21	2:C:385:LEU:HD23	2.01	0.43
1:D:107:ALA:HB2	1:D:240:MET:HE3	2.01	0.43
1:E:168:ASN:ND2	1:E:327:PHE:CE2	2.86	0.43
1:A:225:ARG:NH1	1:A:225:ARG:HA	2.34	0.43
1:A:254:GLU:OE2	1:B:258:ARG:HD3	2.19	0.43
2:C:25:VAL:HG11	2:C:376:PHE:HB2	1.99	0.43
1:D:269:THR:HG21	1:D:279:PHE:H	1.82	0.43
1:E:126:ALA:HB1	1:E:150:ALA:HA	1.99	0.43
1:A:358:ASP:OD2	1:A:360:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ALA:O	1:B:354:ARG:HB2	2.19	0.43
2:C:18:ILE:N	2:C:19:PRO:HD2	2.34	0.43
1:D:109:HIS:CD2	1:D:143:MET:CE	3.01	0.43
1:D:165:SER:HA	1:D:166:PRO:C	2.40	0.43
1:A:309:TYR:HA	1:A:310:PRO:HD2	1.87	0.42
1:B:97:GLY:HA3	1:B:103:LEU:CD1	2.48	0.42
1:E:330:LEU:HG	1:E:331:GLY:N	2.33	0.42
1:F:65:LEU:CD2	1:F:241:VAL:HG21	2.49	0.42
1:A:294:LEU:HG	1:A:306:LEU:HD21	2.02	0.42
1:E:331:GLY:HA2	1:E:360:LYS:O	2.17	0.42
1:F:286:MET:O	1:F:290:ARG:HG3	2.18	0.42
1:B:37:GLU:HG3	1:B:41:LYS:HE3	2.02	0.42
1:E:151:TRP:CD2	1:E:177:VAL:HG11	2.53	0.42
1:F:264:ASN:HA	1:F:267:LYS:HE3	2.00	0.42
2:C:153:PHE:CE2	2:C:155:LYS:HB3	2.55	0.42
2:C:233:ASP:OD1	2:C:233:ASP:C	2.58	0.42
1:F:128:PHE:CZ	1:F:146:TRP:HZ2	2.37	0.42
1:B:100:SER:HB2	1:B:214:THR:HB	2.00	0.42
1:B:127:PRO:HD2	1:B:174:ARG:HH22	1.84	0.42
1:B:165:SER:HB2	1:B:174:ARG:H	1.84	0.42
1:D:322:GLU:HB3	6:D:1045:HOH:O	2.18	0.42
1:D:371:ASP:OD2	1:D:372:VAL:N	2.52	0.42
1:E:275:GLU:HA	1:E:281:LYS:HD3	2.01	0.42
1:B:109:HIS:CD2	1:B:143:MET:HE1	2.54	0.42
1:F:234:LYS:O	1:F:237:ALA:HB3	2.20	0.42
1:D:269:THR:HG23	1:D:279:PHE:H	1.83	0.42
1:E:44:ASP:CG	1:F:51:ARG:NH2	2.72	0.42
1:D:313:PHE:HA	1:D:320:SER:HA	2.02	0.42
1:E:161:GLU:N	1:E:187:LYS:O	2.36	0.42
1:F:78:LYS:HA	1:F:89:THR:HG21	2.02	0.42
1:A:54:ASP:HB3	1:A:55:LEU:HG	2.02	0.42
1:D:159:TYR:CE2	1:D:178:VAL:HG11	2.54	0.42
1:D:55:LEU:HD11	1:D:257:VAL:HG21	2.02	0.41
1:A:343:ARG:NH1	6:A:1101:HOH:O	2.52	0.41
2:C:255:SER:HA	1:D:254:GLU:HG3	2.02	0.41
1:E:150:ALA:O	1:E:151:TRP:CD1	2.63	0.41
1:F:385:LEU:HD23	1:F:386:ILE:CG2	2.49	0.41
1:B:287:MET:HB3	1:B:324:TYR:CB	2.50	0.41
1:D:103:LEU:HG	1:D:229:ALA:HB2	2.02	0.41
1:E:200:THR:OG1	1:E:201:PRO:HD2	2.20	0.41
1:E:194:TYR:CZ	1:E:217:LYS:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:PRO:HD3	1:E:329:TRP:O	2.20	0.41
1:F:103:LEU:HD21	1:F:228:TRP:CA	2.50	0.41
1:F:50:ILE:HD13	1:F:254:GLU:CB	2.50	0.41
1:B:224:SER:O	1:B:255:SER:OG	2.38	0.41
1:F:378:GLU:O	1:F:382:ASN:HB2	2.19	0.41
1:B:219:THR:HG21	1:B:262:ILE:CD1	2.50	0.41
1:D:226:ILE:HG23	1:D:226:ILE:HD12	1.72	0.41
1:D:109:HIS:CD2	1:D:143:MET:HE1	2.56	0.41
1:D:158:PRO:HD3	6:D:1035:HOH:O	2.21	0.41
1:A:48:VAL:HG21	1:A:258:ARG:HG3	2.03	0.41
2:C:156:LYS:H	2:C:156:LYS:HG3	1.27	0.41
1:D:103:LEU:HD12	1:D:103:LEU:HA	1.96	0.41
1:D:112:SER:HA	1:D:120:VAL:HG21	2.02	0.41
1:F:275:GLU:CB	1:F:281:LYS:HD2	2.51	0.41
1:F:331:GLY:HA2	1:F:360:LYS:O	2.20	0.41
1:B:98:THR:HG23	1:B:251:VAL:HG22	2.03	0.41
1:D:225:ARG:CA	1:D:225:ARG:NE	2.84	0.41
1:E:233:ASP:HB3	1:E:236:VAL:HG23	2.02	0.41
1:B:306:LEU:HD12	1:B:306:LEU:HA	1.95	0.41
1:D:112:SER:OG	1:D:144:TYR:HB3	2.20	0.41
1:A:110:ALA:HB1	1:A:239:LYS:HB2	2.03	0.41
1:A:243:TYR:O	1:A:247:ASN:HB2	2.21	0.41
1:B:234:LYS:HE3	1:B:235:GLU:OE2	2.20	0.41
1:E:24:VAL:HG22	1:E:346:LYS:HD3	2.03	0.41
1:A:121:SER:HB3	1:A:147:GLU:HG3	2.02	0.40
1:A:194:TYR:HE2	3:A:1001:PMP:O3	2.04	0.40
1:A:131:THR:O	1:A:135:GLU:HG3	2.20	0.40
1:B:68:PHE:HE1	1:B:245:ILE:CD1	2.34	0.40
2:C:146:TRP:CZ2	2:C:148:GLY:HA2	2.57	0.40
1:B:217:LYS:CG	3:B:1001:PMP:N4A	2.84	0.40
1:B:313:PHE:HA	1:B:320:SER:HA	2.03	0.40
2:C:192:PHE:HB3	2:C:195:TYR:HB3	2.04	0.40
2:C:101:THR:CG2	2:C:217:LLP:OP3	2.69	0.40
2:C:258:ARG:HD3	1:D:254:GLU:OE2	2.21	0.40
2:C:353:GLU:HG2	6:C:480:HOH:O	2.20	0.40
1:E:340:SER:OG	1:E:343:ARG:NH2	2.54	0.40
1:B:192:PHE:HB2	1:B:213:PHE:CE1	2.56	0.40
1:B:234:LYS:HE2	1:B:234:LYS:HB3	1.72	0.40
1:E:123:VAL:HG12	1:E:148:GLY:O	2.21	0.40
1:E:123:VAL:O	1:E:162:LEU:HD23	2.22	0.40
1:F:236:VAL:O	1:F:237:ALA:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:HD12	1:A:314:CYS:SG	2.62	0.40
1:B:271:LYS:HG2	1:B:271:LYS:H	1.77	0.40
1:B:333:LYS:H	1:B:333:LYS:HD2	1.85	0.40
1:D:249:ILE:O	1:D:249:ILE:HG22	2.21	0.40
1:D:258:ARG:O	1:D:262:ILE:HG23	2.21	0.40
1:E:304:PHE:CZ	1:E:385:LEU:HD21	2.57	0.40
1:F:328:ALA:HB3	1:F:364:VAL:HG13	2.03	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	358/391 (92%)	330 (92%)	23 (6%)	5 (1%)	11	7
1	B	367/391 (94%)	345 (94%)	20 (5%)	2 (0%)	29	29
1	D	355/391 (91%)	341 (96%)	14 (4%)	0	100	100
1	E	356/391 (91%)	310 (87%)	39 (11%)	7 (2%)	7	4
1	F	356/391 (91%)	328 (92%)	22 (6%)	6 (2%)	9	4
2	C	356/391 (91%)	331 (93%)	25 (7%)	0	100	100
All	All	2148/2346 (92%)	1985 (92%)	143 (7%)	20 (1%)	17	14

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	LYS
1	B	182	ASP
1	B	183	ASP
1	E	156	LYS
1	E	353	GLU

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Mol	Chain	Res	Type
1	E	386	ILE
1	F	98	THR
1	A	177	VAL
1	A	335	GLU
1	E	157	GLY
1	E	149	ASP
1	A	278	ASN
1	E	162	LEU
1	F	21	SER
1	F	154	ASP
1	F	223	GLY
1	F	302	ASP
1	A	300	GLU
1	E	170	ASP
1	F	218	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/346 (91%)	290 (92%)	25 (8%)	12	10
1	B	322/346 (93%)	296 (92%)	26 (8%)	11	10
1	D	314/346 (91%)	291 (93%)	23 (7%)	14	12
1	E	314/346 (91%)	283 (90%)	31 (10%)	8	5
1	F	314/346 (91%)	291 (93%)	23 (7%)	14	12
2	C	315/345 (91%)	292 (93%)	23 (7%)	14	12
All	All	1894/2075 (91%)	1743 (92%)	151 (8%)	12	10

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	20	MET
1	A	25	VAL

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Mol	Chain	Res	Type
1	A	45	ARG
1	A	80	LEU
1	A	101	THR
1	A	103	LEU
1	A	128	PHE
1	A	134	GLU
1	A	138	TYR
1	A	156	LYS
1	A	184	ASP
1	A	212	LEU
1	A	234	LYS
1	A	255	SER
1	A	269	THR
1	A	295	ARG
1	A	306	LEU
1	A	320	SER
1	A	321	LEU
1	A	322	GLU
1	A	336	THR
1	A	364	VAL
1	A	380	LEU
1	A	382	ASN
1	B	18	ILE
1	B	20	MET
1	B	45	ARG
1	B	80	LEU
1	B	103	LEU
1	B	128	PHE
1	B	134	GLU
1	B	178	VAL
1	B	185	GLU
1	B	212	LEU
1	B	214	THR
1	B	225	ARG
1	B	248	SER
1	B	255	SER
1	B	262	ILE
1	B	269	THR
1	B	284	ARG
1	B	295	ARG
1	B	302	ASP
1	B	306	LEU

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Mol	Chain	Res	Type
1	B	321	LEU
1	B	333	LYS
1	B	364	VAL
1	B	370	GLU
1	B	371	ASP
1	B	380	LEU
2	C	45	ARG
2	C	80	LEU
2	C	101	THR
2	C	103	LEU
2	C	116	ARG
2	C	117	SER
2	C	134	GLU
2	C	138	TYR
2	C	156	LYS
2	C	252	SER
2	C	266	LEU
2	C	269	THR
2	C	281	LYS
2	C	284	ARG
2	C	285	GLU
2	C	295	ARG
2	C	320	SER
2	C	321	LEU
2	C	336	THR
2	C	353	GLU
2	C	371	ASP
2	C	380	LEU
2	C	384	LYS
1	D	20	MET
1	D	23	PHE
1	D	24	VAL
1	D	37	GLU
1	D	80	LEU
1	D	103	LEU
1	D	116	ARG
1	D	121	SER
1	D	123	VAL
1	D	134	GLU
1	D	156	LYS
1	D	212	LEU
1	D	254	GLU

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Mol	Chain	Res	Type
1	D	262	ILE
1	D	267	LYS
1	D	269	THR
1	D	277	GLU
1	D	281	LYS
1	D	321	LEU
1	D	342	LEU
1	D	357	SER
1	D	364	VAL
1	D	380	LEU
1	E	29	HIS
1	E	80	LEU
1	E	83	VAL
1	E	96	VAL
1	E	103	LEU
1	E	123	VAL
1	E	138	TYR
1	E	151	TRP
1	E	161	GLU
1	E	162	LEU
1	E	173	ILE
1	E	187	LYS
1	E	202	ILE
1	E	212	LEU
1	E	255	SER
1	E	258	ARG
1	E	269	THR
1	E	274	SER
1	E	295	ARG
1	E	321	LEU
1	E	323	SER
1	E	332	THR
1	E	338	LEU
1	E	353	GLU
1	E	354	ARG
1	E	357	SER
1	E	361	HIS
1	E	366	MET
1	E	369	ARG
1	E	380	LEU
1	E	385	LEU
1	F	21	SER

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Mol	Chain	Res	Type
1	F	44	ASP
1	F	80	LEU
1	F	98	THR
1	F	103	LEU
1	F	113	SER
1	F	134	GLU
1	F	155	LYS
1	F	225	ARG
1	F	255	SER
1	F	269	THR
1	F	295	ARG
1	F	301	SER
1	F	302	ASP
1	F	306	LEU
1	F	320	SER
1	F	321	LEU
1	F	322	GLU
1	F	364	VAL
1	F	371	ASP
1	F	380	LEU
1	F	385	LEU
1	F	386	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	HIS
1	A	382	ASN
1	B	64	ASN
1	B	382	ASN
2	C	190	HIS
2	C	264	ASN
2	C	345	HIS
2	C	374	ASN
2	C	382	ASN
1	E	167	ASN
1	E	190	HIS
1	E	289	ASN
1	F	64	ASN
1	F	345	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	LLP	C	217	2	23,24,25	2.25	5 (21%)	25,32,34	1.39	4 (16%)

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	LLP	C	217	2	-	8/16/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	217	LLP	C4'-NZ	6.00	1.47	1.27
2	C	217	LLP	C4-C5	5.51	1.48	1.42
2	C	217	LLP	C6-C5	4.37	1.46	1.37
2	C	217	LLP	C4-C4'	2.75	1.51	1.46
2	C	217	LLP	CB-CA	-2.16	1.50	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	217	LLP	C4-C4'-NZ	-3.27	109.29	124.31
2	C	217	LLP	C5'-C5-C6	-3.20	114.11	119.37
2	C	217	LLP	C3-C4-C5	-2.64	116.24	118.26
2	C	217	LLP	C5-C6-N1	-2.49	119.67	123.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	217	LLP	C5'-OP4-P-OP1
2	C	217	LLP	C5'-OP4-P-OP2
2	C	217	LLP	C5'-OP4-P-OP3
2	C	217	LLP	C4-C4'-NZ-CE
2	C	217	LLP	C3-C4-C4'-NZ
2	C	217	LLP	CG-CD-CE-NZ
2	C	217	LLP	CE-CD-CG-CB
2	C	217	LLP	CD-CE-NZ-C4'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	217	LLP	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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$
3	PMP	A	1001	-	16,16,16	2.28	4 (25%)	21,23,23	1.56	5 (23%)
4	PO4	E	1001	-	4,4,4	0.87	0	6,6,6	0.48	0
3	PMP	B	1001	-	16,16,16	2.26	3 (18%)	21,23,23	2.15	8 (38%)

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
3	PMP	A	1001	-	-	2/8/8/8	0/1/1/1
3	PMP	B	1001	-	-	1/8/8/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	PMP	C5-C4	5.66	1.48	1.40
3	A	1001	PMP	C5-C4	5.15	1.47	1.40
3	B	1001	PMP	C3-C4	4.90	1.47	1.40
3	A	1001	PMP	C6-C5	4.88	1.47	1.37
3	B	1001	PMP	C6-C5	4.42	1.47	1.37
3	A	1001	PMP	C3-C4	4.36	1.46	1.40
3	A	1001	PMP	C5A-C5	2.34	1.57	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	PMP	C6-C5-C4	-6.02	113.86	118.12
3	A	1001	PMP	O2P-P-O4P	-3.71	96.85	106.73
3	A	1001	PMP	O3-C3-C2	3.46	125.03	117.49
3	B	1001	PMP	C5A-C5-C6	-3.17	114.15	119.37
3	B	1001	PMP	C6-N1-C2	3.03	124.79	119.17
3	B	1001	PMP	O3-C3-C2	2.65	123.26	117.49
3	B	1001	PMP	C3-C4-C5	2.50	121.12	118.72
3	A	1001	PMP	C6-C5-C4	-2.39	116.43	118.12
3	B	1001	PMP	C4-C4A-N4A	-2.37	103.44	115.38
3	A	1001	PMP	O3P-P-O2P	2.33	116.53	107.64
3	B	1001	PMP	O4P-C5A-C5	-2.29	104.98	109.35
3	A	1001	PMP	C6-N1-C2	2.21	123.26	119.17
3	B	1001	PMP	O3P-P-O4P	-2.08	101.19	106.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	PMP	C5-C4-C4A-N4A
3	A	1001	PMP	C3-C4-C4A-N4A
3	B	1001	PMP	C4-C5-C5A-O4P

There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	PMP	13	0
4	E	1001	PO4	1	0
3	B	1001	PMP	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	362/391 (92%)	0.14	19 (5%)	27	30	24, 45, 70, 88	0
1	B	369/391 (94%)	0.01	15 (4%)	37	40	21, 40, 69, 82	0
1	D	359/391 (91%)	-0.02	12 (3%)	46	48	22, 40, 67, 91	0
1	E	362/391 (92%)	0.47	30 (8%)	11	12	29, 54, 77, 86	0
1	F	360/391 (92%)	0.28	25 (6%)	16	18	26, 49, 75, 88	0
2	C	360/391 (92%)	0.12	15 (4%)	36	38	23, 44, 66, 76	0
All	All	2172/2346 (92%)	0.17	116 (5%)	26	29	21, 45, 72, 91	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	385	LEU	10.2
1	F	385	LEU	9.0
1	E	335	GLU	6.0
1	E	151	TRP	5.9
1	E	150	ALA	5.0
1	D	19	PRO	5.0
1	D	179	ASN	4.8
1	E	274	SER	4.4
1	D	273	GLU	4.4
1	B	274	SER	4.4
2	C	193	ALA	4.3
1	F	151	TRP	4.1
1	A	21	SER	4.0
1	F	154	ASP	4.0
1	A	23	PHE	3.9
1	F	386	ILE	3.9
1	E	153	PHE	3.9
1	D	20	MET	3.8
1	F	157	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	152	GLY	3.8
1	E	273	GLU	3.7
1	A	218	ILE	3.7
1	B	181	PRO	3.7
1	F	273	GLU	3.6
1	F	276	SER	3.6
1	A	185	GLU	3.5
1	E	100	SER	3.5
1	A	193	ALA	3.5
1	A	384	LYS	3.4
2	C	116	ARG	3.4
2	C	274	SER	3.3
1	F	192	PHE	3.3
1	B	302	ASP	3.2
1	F	116	ARG	3.2
2	C	218	ILE	3.2
1	B	180	ARG	3.2
1	F	158	PRO	3.2
1	E	302	ASP	3.2
1	A	214	THR	3.1
1	D	116	ARG	3.1
1	E	162	LEU	3.1
1	F	156	LYS	3.1
1	E	356	GLY	3.1
1	A	215	PHE	3.0
1	D	21	SER	2.9
2	C	153	PHE	2.9
1	F	274	SER	2.9
1	F	153	PHE	2.8
1	E	130	SER	2.8
1	E	178	VAL	2.8
1	E	119	PRO	2.7
2	C	154	ASP	2.7
1	E	339	VAL	2.7
1	D	156	LYS	2.7
2	C	273	GLU	2.7
1	E	276	SER	2.6
1	E	353	GLU	2.6
1	E	115	ALA	2.6
1	B	273	GLU	2.6
1	F	275	GLU	2.6
1	E	214	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	216	SER	2.5
2	C	157	GLY	2.5
1	B	215	PHE	2.5
1	A	18	ILE	2.5
2	C	214	THR	2.5
1	A	20	MET	2.5
1	F	114	LEU	2.5
1	A	116	ARG	2.4
1	F	23	PHE	2.4
2	C	151	TRP	2.4
1	F	177	VAL	2.4
2	C	18	ILE	2.4
1	D	100	SER	2.4
1	F	142	GLY	2.4
1	B	116	ARG	2.4
1	B	179	ASN	2.4
2	C	186	ALA	2.4
1	B	276	SER	2.4
1	D	275	GLU	2.4
1	F	20	MET	2.3
1	E	193	ALA	2.3
1	E	212	LEU	2.3
1	E	228	TRP	2.3
1	E	177	VAL	2.3
1	A	99	GLY	2.3
1	A	226	ILE	2.3
1	B	218	ILE	2.3
1	E	126	ALA	2.3
2	C	177	VAL	2.3
1	E	328	ALA	2.3
1	F	213	PHE	2.2
1	A	100	SER	2.2
1	A	115	ALA	2.2
1	A	22	ASP	2.2
1	F	344	ARG	2.2
1	F	186	ALA	2.2
1	B	214	THR	2.2
1	E	129	TYR	2.2
1	A	213	PHE	2.2
1	F	193	ALA	2.2
1	E	116	ARG	2.2
1	B	183	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	184	ASP	2.1
1	E	19	PRO	2.1
1	D	194	TYR	2.1
1	E	213	PHE	2.1
1	A	227	GLY	2.1
1	F	103	LEU	2.1
2	C	103	LEU	2.1
1	E	103	LEU	2.0
1	D	193	ALA	2.0
1	F	150	ALA	2.0
1	E	343	ARG	2.0
1	B	193	ALA	2.0
1	D	302	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
2	LLP	C	217	24/25	0.95	0.21	41,53,55,58	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
5	PHE	F	2001[B]	12/12	0.88	0.26	29,31,33,35	0
4	PO4	E	1001	5/5	0.94	0.20	61,61,62,62	0
3	PMP	D	1001[A]	16/16	0.94	0.22	48,50,54,57	0
3	PMP	B	1001	16/16	0.95	0.15	54,55,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PMP	A	1001	16/16	0.95	0.20	54,57,60,60	0
3	PMP	F	1001[A]	16/16	0.95	0.18	55,57,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.